



STIC Search Report

EIC 1700

STIC Database Tracking Number: 178325

TO: Dawn Garrett
Location: REM 10C79
Art Unit : 1774
February 1, 2006

Case Serial Number: 10/735732

From: Usha Shrestha
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-3519
usha.shrestha@uspto.gov

Search Notes

Examiner Garrett,

For the answer set L44 there are 198 hit Registry Number so I used fhistr (First Hit Structure) command to print the transcript. If you have any questions please let me know. Thank you.

/

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: DAVID GARRETT Examiner #: 76107 Date: 2/1/2006
 Art Unit: 1774 Phone Number 302-1523 Serial Number: 10/735,732
 Mail Box and Bldg/Room Location: Room 10C79 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Light Emitting Device and a Method of Manufacturing There

Inventors (please provide full names): Atsushi Tokuda, Takako Takasu,
Satoshi Seo, Ryoji Nomura

Earliest Priority Filing Date: 12/19/02 (Japan 2002-368692)

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search the conjugate polymer material of claim 1 wherein the fundamental skeleton is polythiophene and the electron-accepting organic compound is one of formulas (2) to (9) (see cl. 7).

If few hits are obtained, please expand the search to the other conjugate polymers listed in claim 1, which are the following:
 polyanilines, polypyrrole, and polyfuran.

SCIENTIFIC REFERENCE BR
 Sci & Tech Inf. Ctr.

FEB 1 2006 REC'D

Pat. & T.M. Office

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>Wika</u>	NA Sequence (#) _____	STN <u>385.63</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit _____
Date Searcher Picked Up: <u>2/1/06</u>	Bibliographic _____	Dr.Link _____
Date Completed: <u>2/1/06</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>60</u>	Fulltext <input checked="" type="checkbox"/>	Sequence Systems _____
Clerical Prep Time: <u>30</u>	Patent Family _____	WWW/Internet _____
Online Time: <u>150</u>	Other _____	Other (specify) _____

=> fil reg

FILE 'REGISTRY' ENTERED AT 15:10:34 ON 01 FEB 2006

=> d his ful

FILE 'HCAPLUS' ENTERED AT 12:44:52 ON 01 FEB 2006

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FILE 'REGISTRY' ENTERED AT 12:45:16 ON 01 FEB 2006

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118-75-2/BI OR 122721-91-9/BI OR 122721-92-0/BI OR
123-93-3/BI OR 1518-16-7/BI OR 1822-66-8/BI OR
211235-81-3/BI OR 228721-87-7/BI OR 27728-29-6/BI OR
527-21-9/BI OR 613-20-7/BI OR 64-17-5/BI OR 670-54-2/BI
OR 725246-76-4/BI OR 74-96-4/BI OR 925-47-3/BI)

L3 1 SEA ABB=ON PLU=ON 106-51-4/RN

L4 1 SEA ABB=ON PLU=ON 118-75-2/RN

L5 1 SEA ABB=ON PLU=ON 527-21-9/RN

L6 1 SEA ABB=ON PLU=ON 613-20-7/RN

L7 1 SEA ABB=ON PLU=ON 670-54-2/RN

L8 1 SEA ABB=ON PLU=ON 1518-16-7/RN

L9 1 SEA ABB=ON PLU=ON 27728-29-6/RN

L10 1 SEA ABB=ON PLU=ON 725246-76-4/RN

L11 537066 SEA ABB=ON PLU=ON 16.145/RID

L12 5 SEA ABB=ON PLU=ON L2 AND L11

L13 8210 SEA ABB=ON PLU=ON L11 AND PMS/CI

L14 2 SEA ABB=ON PLU=ON L2 AND L13

L15 8 SEA ABB=ON PLU=ON (L3 OR L4 OR L5 OR L6 OR L7 OR L8
OR L9 OR L10)

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L17 11341 SEA ABB=ON PLU=ON L13

L18 100 SEA ABB=ON PLU=ON L16 AND L17

L19 18 SEA ABB=ON PLU=ON L18 AND OPTIC?/SC,SX

L20 1 SEA ABB=ON PLU=ON L19 AND L1

FILE 'REGISTRY' ENTERED AT 14:00:12 ON 01 FEB 2006

L21 3 SEA ABB=ON PLU=ON L12 NOT L14

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L22 47 SEA ABB=ON PLU=ON L21

L23 1 SEA ABB=ON PLU=ON L22 AND L16

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L25 491649 SEA ABB=ON PLU=ON L24 NOT L13

L26 40622 SEA ABB=ON PLU=ON L25 AND 1/NR

L27 451027 SEA ABB=ON PLU=ON L25 NOT L26

L28 451027 SEA ABB=ON PLU=ON L27 OR L27

D RN 250000

L29 250000 SEA RAN=(372106-72-4,) ABB=ON PLU=ON L27 OR L27

L30 201027 SEA ABB=ON PLU=ON L28 NOT L29

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L31 12110 SEA ABB=ON PLU=ON L29

L32 66784 SEA ABB=ON PLU=ON L30

L33 47710 SEA ABB=ON PLU=ON L26

L34 97518 SEA ABB=ON PLU=ON (L31 OR L32 OR L33)

L35 393 SEA ABB=ON PLU=ON L34 AND L16
 L36 45 SEA ABB=ON PLU=ON L35 AND OPTIC?/SC,SX
 L37 55 SEA ABB=ON PLU=ON L19 OR L36
 L38 8 SEA ABB=ON PLU=ON L37 AND (HOLE(2A)TRANSPORT? OR
 LIGHT(2A) (EMIT? OR EMISSION?) OR ELECTROLUMINE? OR
 LUMINE? OR ORGANOLUM!N? OR EL OR E(W)L OR L(W)E(W)D)
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 L40 12 SEA ABB=ON PLU=ON L39 AND P/DT
 L41 9 SEA ABB=ON PLU=ON L40 AND (1907-2002)/PRY,AY
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 L44 43 SEA ABB=ON PLU=ON L41 OR L43

=> d que 144

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 L5 1 SEA FILE=REGISTRY ABB=ON PLU=ON 527-21-9/RN
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 L31 12110 SEA FILE=HCAPLUS ABB=ON PLU=ON L29
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 L33 47710 SEA FILE=HCAPLUS ABB=ON PLU=ON L26
 L34 97518 SEA FILE=HCAPLUS ABB=ON PLU=ON (L31 OR L32 OR L33)
 L35 393 SEA FILE=HCAPLUS ABB=ON PLU=ON L34 AND L16
 L36 45 SEA FILE=HCAPLUS ABB=ON PLU=ON L35 AND OPTIC?/SC,SX
 L37 55 SEA FILE=HCAPLUS ABB=ON PLU=ON L19 OR L36
 L38 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND (HOLE(2A)TRANS
 PORT? OR LIGHT(2A) (EMIT? OR EMISSION?) OR ELECTROLUMINE
 ? OR LUMINE? OR ORGANOLUM!N? OR EL OR E(W)L OR
 L(W)E(W)D)
 L39 55 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 OR L38
 L40 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND P/DT
 L41 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L40 AND (1907-2002)/PR
 Y,AY
 L42 43 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 NOT L40
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 L44 43 SEA FILE=HCAPLUS ABB=ON PLU=ON L41 OR L43

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FILE 'HCAPLUS' ENTERED AT 15:11:07 ON 01 FEB 2006

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E462 THROUGH E660 ASSIGNED

=> d 144 1-43 ibib abs fhitr hitind

L44 ANSWER 1 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:589795 HCAPLUS
DOCUMENT NUMBER: 141:147851
TITLE: **Light-emitting** device and
method for manufacturing same
INVENTOR(S): Tokuda, Atsushi; Takasu, Takako; Seo, Satoshi;
Nomura, Ryoji
PATENT ASSIGNEE(S): Semiconductor Energy Laboratory Co., Ltd.,
Japan
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004062322	A1	20040722	WO 2003-JP15766	

2003
1210

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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,
CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG,
ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT,
RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT,
TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY,
CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA,
GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004241492	A1	20041202	US 2003-735732
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2003
1216

PRIORITY APPLN. INFO.:

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JP 2002-368692

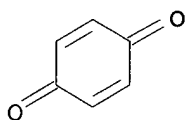
A

2002
1219

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AB A conjugated polymer which has a basic skeleton of a polythiophene derivative, a polyaniline derivative, a polypyrrole derivative, or a polyfuran derivative and is soluble to organic compds. is doped with a dopant that is an electron-accepting organic mol. not containing an acid component for oxidization of the main chain. An El device of the present invention is characterized by using such a doped conjugated polymer as a material for a hole injection layer. Since this polymer is soluble to organic solvents, a film thereof can be

formed on a highly H₂O-repellent substrate through application. Therefore, a film thereof can be easily formed on a TFT substrate which is necessary to an active matrix display. Since a dopant not containing an acid component is used, influences on an organic thin film or an electrode which is in contact with the hole injection layer can be suppressed to the min.

IT 106-51-4, p-Quinone, uses
 (doped in polythiophenes; **hole transport**
 material for **light-emitting** device and
 display)
 RN 106-51-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



IC ICM H05B033-14
 ICS H05B033-22
 CC 73-11 (Optical, Electron, and Mass Spectroscopy and
 Other Related Properties).
 Section cross-reference(s): 38, 74
 ST **light emitting** device manufg polythiophene
hole transport display
 IT **Electroluminescent** devices
 (displays; **hole transport** material for
light-emitting device and display)
 IT Polyanilines
 (doped with electron accepting organic compound; **hole**
transport material for **light-emitting**
 device and display)
 IT **Luminescent** screens
 (electroluminescent; **hole transport**
 material for **light-emitting** device and
 display)
 IT Coating materials
 Coating process
Electroluminescent devices
 (**hole transport** material for **light**
-emitting device and display)
 IT **Hole transport**
 (material; **hole transport** material for
light-emitting device and display)
 IT Conducting polymers
 (polyfurans, doped with electron accepting organic compound;
hole transport material for **light-**
emitting device and display)
 IT Conducting polymers
 (polypyrroles, doped with electron accepting organic compound;
hole transport material for **light-**
emitting device and display)
 IT Conducting polymers
 (polythiophenes, doped with electron accepting organic compound;
hole transport material for **light-**
emitting device and display)
 IT 106-51-4, p-Quinone, uses 118-75-2,
 Tetrachloro-p-quinone, uses 527-21-9,

Tetrafluoro-p-quinone 613-20-7, 2,6-Naphthoquinone
670-54-2, TCNE, uses 1518-16-7, TCNQ
27728-29-6 725246-76-4

(doped in polythiophenes; hole transport
material for light-emitting device and
display)

IT 122721-92-0 228721-87-7

(doped with electron accepting organic compds.; hole
transport material for light-emitting
device and display)

IT 64-17-5, Ethanol, reactions 74-96-4, Ethylbromide 111-25-1,
1-Bromohexane 123-93-3, Thiodiglycolic acid

(hole transport material for light
-emitting device and display)

IT 925-47-3P 1822-66-8P, 2,5-Diethoxycarbonyl-3,4-
dihydroxythiophene 122721-91-9P 211235-81-3P

(hole transport material for light
-emitting device and display)

L44 ANSWER 2 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:1004473 HCAPLUS

DOCUMENT NUMBER: 140:10361

TITLE: Nondegenerate four-wave mixing using
photoinduced charge-transfer materials

INVENTOR(S): Maniloff, Eric S.; McBranch, Duncan W.;
Heeger, Alan J.; Vacar, Dan V.

PATENT ASSIGNEE(S): The Regents of the University of California,
USA

SOURCE: U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part
of U.S. Ser. No. 889,787, abandoned.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

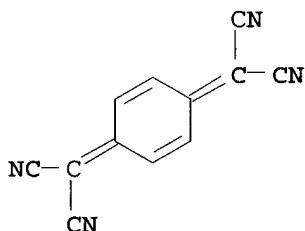
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2002114998	A1	20020822	US 2001-973170	2001 1004
			<--	
US 6761999	B2	20040713		
PRIORITY APPLN. INFO.:			US 1996-16093P	P 1996 0708
			<--	
			US 1997-889787	B2 1997 0708
			<--	

AB Methods for nondegenerate four-wave mixing in charge-transfer
materials are described which comprise preparing a mixture of a
semiconducting polymer charge-donor species with a charge-acceptor
species between which charge transfer occurs in the absence of an
externally applied d.c. elec. field when the mixture is excited by
light within a wavelength region which is absorbed by the
charge-donor species; exciting the mixture with two pulsed light
beams within the wavelength region, the two pulsed light beams

intersecting each other at an angle in the mixture, each of the beams having a pulse width less than the time required for charge to be transferred back from the charge-acceptor species to the charge-donor species, so that a holog. grating is formed in the region of the mixture surrounding the intersection of the beams; passing light within a second wavelength region through the holog. grating region of the blend, wherein the light within the second wavelength region is chosen so as not to be absorbed by the mixture in the absence of charge transfer; and detecting the diffracted light within the second wavelength region.

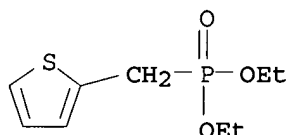
IT 1518-16-7D, Tetracyano-p-quinodimethane, derivs.
(nondegenerate four-wave mixing using photoinduced charge-transfer materials)
RN 1518-16-7 HCAPLUS
CN Propanedinitrile, 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis-(9CI) (CA INDEX NAME)



IC ICM G03H001-02
ICS G03H001-04
INCL 430001000; 430002000; 359003000
CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
IT 1518-16-7D, Tetracyano-p-quinodimethane, derivs.
99685-96-8, [5,6]Fullerene-C60-Ih
(nondegenerate four-wave mixing using photoinduced charge-transfer materials)
IT 574-93-6D, Phthalocyanine, derivs. 104934-50-1, Poly(3-hexyl thiophene)
(nondegenerate four-wave mixing using photoinduced charge-transfer materials)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 3 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:965533 HCAPLUS
DOCUMENT NUMBER: 138:287249
TITLE: Dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices
AUTHOR(S): Jen, Alex K. Y.; Luo, Jingdong; Ma, Hong; Haller, Marnie; Barto, Richard R.; Frank, Curtis W.
CORPORATE SOURCE: Department of Materials Science and Engineering, Univ. of Washington, Seattle, WA, 98195-2120, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (2002), 4809(Nanoscale Optics and Applications), 79-85

CODEN: PSISDG; ISSN: 0277-786X
 PUBLISHER: SPIE-The International Society for Optical Engineering
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Encapsulated by highly-fluorinated dendrons, a nonlinear optical chromophore core, which is based on the phenyl-tetracyanobutadienyl (Ph-TCBD) thiophene-stilbene-based NLO chromophore, exhibits a large .apprx.30-40 nm blue shift of the charge-transfer absorption maximum, 20° higher decomposition temperature, and most impressively, three times higher E-O coefficient. The combination of these appreciable improvements makes the mol. design of dendritic modification as a very promising mol.-engineering for next generation of E-O materials.
 IT 2026-42-8 (Wittig type olefination in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 RN 2026-42-8 HCAPLUS
 CN Phosphonic acid, (2-thienylmethyl)-, diethyl ester (9CI) (CA INDEX NAME)



CC 22-13 (Physical Organic Chemistry)
 Section cross-reference(s): 73
 IT 2026-42-8 (Wittig type olefination in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 IT 507234-08-4P (Wittig type olefination in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 IT 670-54-2, TCNE, reactions (conversion to FLDR by reaction with TCNE; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 IT 445421-40-9P (conversion to FLDR by reaction with TCNE; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 IT 220127-22-0 (dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 IT 507234-11-9P (esterification in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)
 IT 507234-10-8

(iodination in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)

IT 507234-09-5P

(iodination in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)

IT 445421-43-2P

(saponification in conversion to synthetic intermediate for preparation of chromophore; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)

IT 445421-40-9DP, polymer

(spectral matrix medium; dendritic NLO chromophore with fluorinated dendrons for improving poling efficiency in electro-optic devices)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 4 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:348262 HCAPLUS

DOCUMENT NUMBER: 137:79010

TITLE: Preparation of 4,4-Diaryl-2-(tricyanoethenyl)dithienosiloles and Vapor - Chromic Behavior of the Film

AUTHOR(S): Ohshita, Joji; Lee, Kwang-Hoi; Hashimoto, Mimi; Kunugi, Yoshihito; Harima, Yutaka; Yamashita, Kazuo; Kunai, Atsutaka

CORPORATE SOURCE: Institute for Fundamental Research of Organic Chemistry, Kyushu University, Fukuoka, 812-8581, Japan

SOURCE: Organic Letters (2002), 4(11), 1891-1894
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

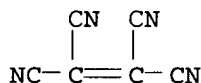
OTHER SOURCE(S): CASREACT 137:79010

AB Reactions of 4,4-diphenyl- and 4,4-di(p-tolyl)dithienosilole with tetracyanoethene (TCNE) in DMF gave coupling products 4,4-diphenyl- and 4,4-di(p-tolyl)-2-(tricyanoethenyl)dithienosilole (1a and 1b) in good yield. The films of 1b exhibited vapor-chromism, and the color of the film changed from red to blue-purple upon exposure to the vapor of organic solvents such as ethanol, methanol, acetonitrile, Et acetate, acetone, and hexane. The color reverted to the original red upon contact with chloroform vapor, indicating that this process is reversible.

IT 670-54-2, Tetracyanoethene, reactions
(alkylation of diaryldithienosilole with)

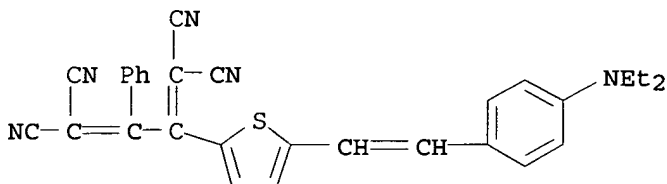
RN 670-54-2 HCAPLUS

CN Ethenetetracarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 72, 73
 ST diaryl tricyanoethenyl dithienosilole prepn vapor chromic behavior
 film; aryl cyanoethyl dithienosilole prepn vapor chromic behavior
 film; HOMO LUMO **luminescence** optical electrochem
 property tricyanoethenyl dithienosilole thiophene
 IT **Luminescence**
 (of diaryl(tricyanoethenyl)dithienosiloles)
 IT 670-54-2, Tetracyanoethene, reactions
 (alkylation of diaryldithienosilole with)
 IT 492-97-7, 2,2'-Bithiophene
 (alkylation with tetracyanoethene)
 IT 440669-03-4P 440669-05-6P 440669-07-8P
 (preparation and optical and electrochem. property of)
 REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L44 ANSWER 5 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2002:270343 HCAPLUS
 DOCUMENT NUMBER: 137:160692
 TITLE: Large electro-optic activity and low optical
 loss derived from a highly fluorinated
 dendritic nonlinear optical chromophore
 AUTHOR(S): Luo, Jingdong; Ma, Hong; Haller, Marnie; Jen,
 Alex K.-Y.; Barto, Richard R.
 CORPORATE SOURCE: Department of Materials Science and
 Engineering, University of Washington,
 Seattle, WA, 98195-2120, USA
 SOURCE: Chemical Communications (Cambridge, United
 Kingdom) (2002), (8), 888-889
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A 3-dimensional shape nonlinear optical chromophore encapsulated
 by highly-fluorinated dendrons exhibits significantly improved
 electrooptic properties and optical attenuation.
 IT 220127-22-0P
 (large electro-optic activity and low optical loss derived from
 a highly fluorinated dendritic nonlinear optical chromophore)
 RN 220127-22-0 HCAPLUS
 CN 1,3-Butadiene-1,1,4,4-tetracarbonitrile, 2-[5-[2-[4-
 (diethylamino)phenyl]ethenyl]-2-thienyl]-3-phenyl- (9CI) (CA
 INDEX NAME)



CC 73-2 (Optical, Electron, and Mass Spectroscopy and Other
 Related Properties)
 Section cross-reference(s): 69, 76
 IT 220127-22-0P 445421-40-9P

(large electro-optic activity and low optical loss derived from
a highly fluorinated dendritic nonlinear optical chromophore)
IT 670-54-2, TCNE, reactions 445421-41-0
445421-43-2

(large electro-optic activity and low optical loss derived from
a highly fluorinated dendritic nonlinear optical chromophore)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L44 ANSWER 6 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:804097 HCAPLUS

DOCUMENT NUMBER: 136:85772

TITLE: Synthesis and Properties of an Aggregating
Heterocyclic Helicene

AUTHOR(S): Phillips, Karen E. S.; Katz, Thomas J.;
Jockusch, Steffen; Lovinger, Andrew J.; Turro,
Nicholas J.

CORPORATE SOURCE: Department of Chemistry, Columbia University,
New York, NY, 10027, USA

SOURCE: Journal of the American Chemical Society
(2001), 123(48), 11899-11907
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:85772

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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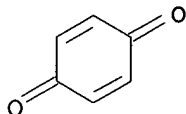
AB Heterohelicene I is synthesized in six steps from 3,3'-bithienyl.
Because the number of steps is small, because the yield is 95% in the
last (the reaction of a bis-enol ether with 1,4-benzoquinone, a
six-step one pot procedure that constructs the helicene skeleton),
and because chromatog. is not required to purify any of the
products in the synthesis, significant amts. are easily prepared To
convert I into enantiopure helicene II, a helicenebisquinone
surrounded by four dodecyloxy groups, requires only a precededented
three-step sequence. Enantiopure II, either without solvent or in
dodecane (but not in chloroform) aggregates into columnar
structures whose optical properties differ markedly from those of
the monomer but resemble those shown previously only by aggregates
of its benzo analog. Evidence of aggregation in the pure material
includes optical microscopic observation of long fibrous
structures and X-ray diffraction and combined transmission
electron microscopic and electron diffraction analyses showing the
mols. within the fibers to be organized in columnar arrays. The
CD spectra, sp. rotations, and fluorescent emission spectra of the
aggregated structures are all distinctive, and, as reported
elsewhere, the second harmonic response is very large. The linear
polarizations of the monomers' and aggregates' fluorescent
emissions differ greatly. The circular polarization of the
aggregates' fluorescent emission, after excitation by unpolarized
light, is large.

IT 106-51-4, p-Benzoquinone, reactions

(synthesis and properties of an aggregating heterocyclic
helicene)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 73, 75, 76

IT 106-51-4, p-Benzoquinone, reactions 3172-56-3,

3,3'-Bithiophene 4292-19-7, 1-Iodododecane

(synthesis and properties of an aggregating heterocyclic
helicene)

REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L44 ANSWER 7 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:315858 HCAPLUS

DOCUMENT NUMBER: 135:92463

TITLE: Synthesis and Photoisomerization of
Dithienylethene-Bridged Diporphyrins

AUTHOR(S): Osuka, Atsuhiko; Fujikane, Daisuke; Shinmori,
Hideyuki; Kobatake, Seiya; Irie, Masahiro

CORPORATE SOURCE: Department of Chemistry Graduate School of
Science, Kyoto University and CREST Japan
Science Technology Corporation (JST), Kyoto,
606-8502, Japan

SOURCE: Journal of Organic Chemistry (2001), 66(11),
3913-3923

CODEN: JOCEAH; ISSN: 0022-3263

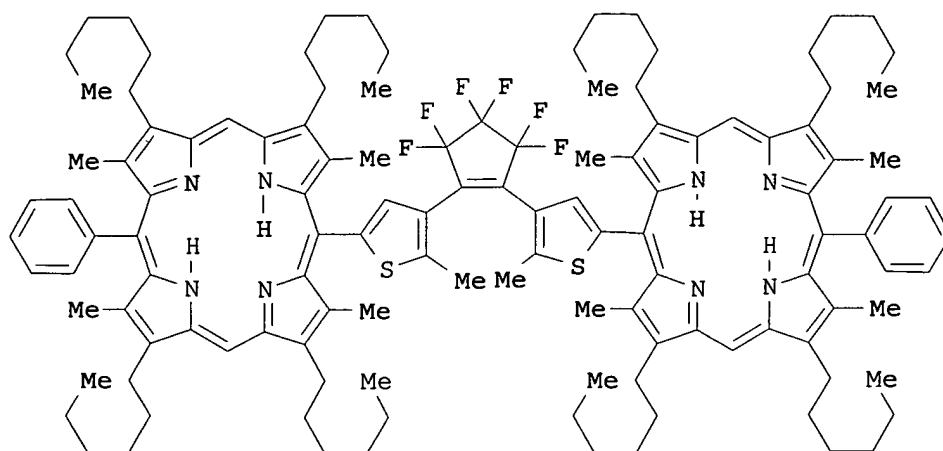
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:92463

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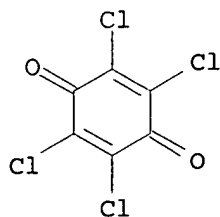
I

AB Dithienylethene-bridged diporphyrins, e.g. I, were prepared as photochem. switching mols. The close attachment of the porphyrin chromophore to the dithienylethene led to the loss of their photochromic reactivity, and therefore some examples did not undergo any photochem. isomerization, probably due to efficient quenching of the excited dithienylethene by the attached porphyrin moiety via intramol. energy transfer. The pertinent insertion of a spacer between the dithienylethene and porphyrin moieties allowed two examples to undergo open-to-closed and closed-to-open photoisomerizations in quantum yields of 4.3×10^{-2} and 1.8×10^{-3} , and 2.6×10^{-3} and 7.5×10^{-4} , resp., by irradiation with 313 and 625 nm light, which are considerably smaller than quantum yields of 0.52 and 3.8×10^{-3} for a reference dithienylethene. The fluorescence of one example was regulated in a reversible manner by the photoisomerization of the dithienylethene moiety. In addition, the absorption properties of the porphyrin in another example changed in response to the photochromic reaction of the dithienylethene bridge.

IT 118-75-2, p-Chloranil, reactions
(preparation of)

RN 118-75-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro- (9CI) (CA
INDEX NAME)



CC 26-7 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 73, 74

IT 76-03-9, Trichloroacetic acid, reactions 118-75-2,
p-Chloranil, reactions 557-34-6, Zinc acetate 603-32-7
(preparation of)

IT 348638-91-5P
(synthesis and photoisomerization of dithienylethene-bridged
diporphyrins)

IT 348638-85-7P 348638-87-9P 348638-89-1P
348638-93-7P 348638-95-9P 348639-10-1P
348639-36-1P 348639-40-7P
(synthesis and photoisomerization of dithienylethene-bridged
diporphyrins)

IT 100-52-7, Benzaldehyde, reactions 126-30-7 559-40-0,
Octafluorocyclopentene 1066-54-2, Trimethylsilylacetylene
29421-73-6 29421-75-8 126136-05-8
134856-58-9 154566-69-5 226083-60-9
348639-12-3 348639-29-2 348639-38-3
(synthesis and photoisomerization of dithienylethene-bridged
diporphyrins)

IT 154566-75-3P 348638-97-1P 348639-00-9P
348639-02-1P 348639-05-4P 348639-14-5P
348639-16-7P 348639-20-3P 348639-25-8P
348639-27-0P 349498-91-5P
(synthesis and photoisomerization of dithienylethene-bridged
diporphyrins)

IT 348639-08-7P 349542-93-4P 349542-97-8P
(synthesis and photoisomerization of dithienylethene-bridged
diporphyrins)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L44 ANSWER 8 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:375984 HCAPLUS

DOCUMENT NUMBER: 133:58482

TITLE: Basis set dependence of the vibrational
wavenumbers of the out-of-plane modes of
conjugated π -electron ring systems

AUTHOR(S): Torii, H.; Ishikawa, A.; Takashima, R.;
Tasumi, M.

CORPORATE SOURCE: School of Science, Department of Chemistry,
The University of Tokyo, Tokyo, 113-0033,
Japan

SOURCE: THEOCHEM (2000), 500, 311-321
CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

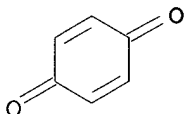
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Basis set dependence of the vibrational wavenumbers of
out-of-plane modes calculated at the MP2 level of ab initio MO theory
is examined for benzene, p-benzoquinodimethane, p-benzoquinone,
furan, and thiophene. Various polarization functions up to
(3df,p) are used in combination with the 6-31G and 6-311G basis
sets. Especially in the case of normal modes with alternate
out-of-plane motions of the C atoms (such as the ν_4 (b_{2g}) mode
of benzene), the calculated wavenumbers depend strongly on the
exponents (α_d) of the d. functions on the C atoms. It is
therefore necessary to include d. functions with an optimum
exponent ($\alpha_d \text{ simeq } 0.4$) on the C atoms to obtain reasonable
out-of-plane vibrational force fields. In a few cases (such as
the ν_{16} (a_2) mode of furan), inclusion of a set of f functions

on the C atoms has some effects on the calculated wavenumbers of out-of-plane modes. However, unless the basis set contains an optimum set of d. functions, inclusion of a set of f functions does not improve the agreement between the observed and calculated vibrational wavenumbers. As a case with an exaggerated effect of basis set, the wavenumber of the ν_{41} (b_{2g}) mode of the planar optimized structure of p-benzoquinodimethane is imaginary by using the 6-311G(d,p) or 6-311G(df,p) basis set at the MP2 level. For all the mols. treated reasonable out-of-plane vibrational force fields are obtained by using the 6-31G(2df,p) and 6-311G(2df,p) basis sets.

IT 106-51-4, p-Benzoquinone, properties
(basis set dependence of vibrational wave nos. of out-of-plane modes of conjugated π -electron ring systems)
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)
Section cross-reference(s): 73
IT 71-43-2, Benzene, properties 106-51-4, p-Benzoquinone,
properties 110-00-9, Furan 110-02-1, Thiophene
502-86-3, p-Benzoquinodimethane
(basis set dependence of vibrational wave nos. of out-of-plane modes of conjugated π -electron ring systems)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

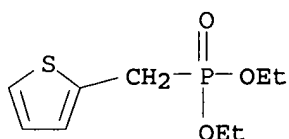
L44 ANSWER 9 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:70296 HCAPLUS
DOCUMENT NUMBER: 132:194763
TITLE: A nonlinear optical polyurethane
functionalized with a heteroaromatic thiophene
ring having a tricyanovinyl group
AUTHOR(S): Woo, Han Young; Shim, Hong-Ku; Lee, Kwang-Sup
CORPORATE SOURCE: Department of Chemistry, Korea Advanced
Institute of Science and Technology, Taejeon,
305-701, S. Korea
SOURCE: Polymer Journal (Tokyo) (2000), 32(1), 8-14
CODEN: POLJB8; ISSN: 0032-3896
PUBLISHER: Society of Polymer Science, Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new functionalized polyurethane structure with a thiophene ring
having a tricyanovinyl group in the polymer side chain was
synthesized. The mol. weight of the final polymer was $M_n = 12,000$
and $M_w/M_n = 2.04$. The resulting polymer was soluble in
N-methylpyrrolidinone and could be processed into good optical
quality films by spin casting at ca. 100°C. It showed no
weight loss up to 266°C in the thermogravimetric anal. and a
definite glass transition at 176°C. The second-order
nonlinear optical coefficient, d_{33} , was determined to be 51 pm V⁻¹ from
measuring the second harmonic generation (SHG) for a thin polymer

film after poling treatment. The outstanding orientational stability of the aligned chromophores was observed up to about 150°C, which originated from the rigid polymer backbone and the stabilizing function of the hydrogen bridges formed between the neighboring polyurethane chains.

IT 2026-42-8P, Diethyl 2-thienylmethylphosphonate
(monomer intermediate; preparation of nonlinear optical polyurethane containing tricyanovinylthiophene groups)

RN 2026-42-8 HCAPLUS

CN Phosphonic acid, (2-thienylmethyl)-, diethyl ester (9CI) (CA INDEX NAME)



CC 35-5 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 36, 38, 73

IT 2026-42-8P, Diethyl 2-thienylmethylphosphonate
19249-34-4P, N,N-Bis(2-acetoxyethyl)aniline 41313-77-3P,
4-[Bis(2-acetoxyethyl)amino]benzaldehyde 45438-73-1P,
2-(Bromomethyl)thiophene
(monomer intermediate; preparation of nonlinear optical polyurethane containing tricyanovinylthiophene groups)

IT 68-12-2, DMF, reactions 108-24-7, Acetic anhydride 120-07-0,
N,N-Bis(2-hydroxyethyl)aniline 122-52-1, Triethyl phosphite
554-14-3, 2-Methylthiophene
(monomer starting material; preparation of nonlinear optical polyurethane containing tricyanovinylthiophene groups)

IT 195058-35-6P
(monomer; preparation of nonlinear optical polyurethane containing tricyanovinylthiophene groups)

IT 213741-94-7P 213741-95-8P
(polymer intermediate; preparation of nonlinear optical polyurethane containing tricyanovinylthiophene groups)

IT 670-54-2DP, Tetracyanoethylene, reaction products with
polyurethane thienylvinyl derivs. 213741-94-7DP,
reaction products with tetracyanoethylene 213741-95-8DP,
reaction products with tetracyanoethylene
(preparation of nonlinear optical polyurethane containing tricyanovinylthiophene groups)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L44 ANSWER 10 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:55923 HCAPLUS

DOCUMENT NUMBER: 132:180499

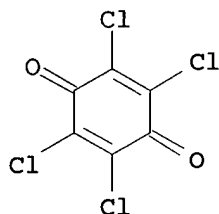
TITLE: Search for new luminophores with predetermined
physicochemical and chemical properties. I.
1,3,5-Triarylpyrazoles

AUTHOR(S): Shkumat, A. P.

CORPORATE SOURCE: Ukraine

SOURCE: Visnik Kharkivs'kogo Universitetu (1998),
(2(Chem.)), 121-125
CODEN: VKSGA3; ISSN: 0453-8048

PUBLISHER: Kharkivs'kii Derzhavnii Universitet
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 AB The luminophores 1,5-diphenyl-3-arylpyrazoles were prepared by reaction of the corresponding pyrazolines with nickel peroxide. Absorption and **luminescence** spectra of the obtained luminophores are discussed.
 IT 118-75-2, Chloranil, uses
 (triarylpyrazole luminophores with improved stability prepared from corresponding pyrazolines)
 RN 118-75-2 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro- (9CI) (CA INDEX NAME)



CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 73
 IT Dehydrogenation
 Fluorescence
 IR absorption
 Luminescent substances
 (triarylpyrazole luminophores with improved stability prepared from corresponding pyrazolines)
 IT 118-75-2, Chloranil, uses 1313-13-9, Manganese dioxide, uses
 (triarylpyrazole luminophores with improved stability prepared from corresponding pyrazolines)
 IT 742-01-8 1450-62-0 2256-23-7 2515-49-3 2755-70-6
 10180-02-6 13393-39-0 13393-41-4 **16723-77-6**
 19429-34-6 22948-37-4 **259665-24-2**
 (triarylpyrazole luminophores with improved stability prepared from corresponding pyrazolines)
 IT 2183-27-9P, 1,3,5-Triphenylpyrazole 12035-36-8P, Nickel oxide (NiO2) 16112-34-8P 16901-34-1P **21178-99-4P**
 27293-95-4P 33045-40-8P 259665-15-1P 259665-16-2P
 259665-17-3P 259665-19-5P 259665-21-9P 259665-22-0P
 (triarylpyrazole luminophores with improved stability prepared from corresponding pyrazolines)

L44 ANSWER 11 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1999:459290 HCAPLUS
 DOCUMENT NUMBER: 131:200158
 TITLE: A new NLO polyurethane with a tricyanovinyl group
 AUTHOR(S): Woo, Han Young; Shim, Hong-Ku; Lee, Kwang-Sup
 CORPORATE SOURCE: Department of Chemistry, Korea Advanced Institute of Science and Technology, Taejon, 305-701, S. Korea
 SOURCE: Synthetic Metals (1999), 101(1-3), 136-137
 CODEN: SYMEDZ; ISSN: 0379-6779

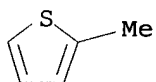
PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A new functionalized polyurethane structure with a heteroarom. thiophene ring having a tricyanovinyl group in the polymer side chain was synthesized. The resulting polymer was soluble in N-methylpyrrolidinone and could be processed into good optical quality films by spin casting at ca. 100 °C. The second-order nonlinear coefficient, d_{33} , was determined to be 51 pm/V from measuring the second harmonic generation (SHG) for a thin polymer film. The outstanding orientational stability of the aligned chromophores was observed up to about 150°C, which originated from the rigid polymer backbone and the stabilizing function of the hydrogen bridges formed between the neighboring polyurethane chains.

IT 554-14-3, 2-Methylthiophene
 (in monomer preparation; nonlinear optical polyurethanes containing (tricyanovinyl)thiophenyl groups in side chains)

RN 554-14-3 HCAPLUS

CN Thiophene, 2-methyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 35-5 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 73

IT 122-52-1, Triethyl phosphite 128-08-5, N-Bromosuccinimide
 554-14-3, 2-Methylthiophene 2026-42-8
 41313-77-3
 (in monomer preparation; nonlinear optical polyurethanes containing (tricyanovinyl)thiophenyl groups in side chains)

IT 45438-73-1P, 2-Bromomethylthiophene
 (in monomer preparation; nonlinear optical polyurethanes containing (tricyanovinyl)thiophenyl groups in side chains)

IT 195058-35-6P
 (monomer; nonlinear optical polyurethanes containing (tricyanovinyl)thiophenyl groups in side chains)

IT 670-54-2DP, Tetracyanoethylene, reaction products with N,N-bis(2-hydroxyethyl)-4-[(2-thiophen-2-yl)vinyl]aniline-4,4'-diisocyanato-3,3'-dimethoxybiphenyl copolymer
 213741-94-7DP, reaction products with tetracyanoethylene
 213741-95-8DP, reaction products with tetracyanoethylene
 (nonlinear optical polyurethanes containing (tricyanovinyl)thiophenyl groups in side chains)

IT 213741-94-7P 213741-95-8DP, reaction products with tetracyanoethylene
 (nonlinear optical polyurethanes containing (tricyanovinyl)thiophenyl groups in side chains)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

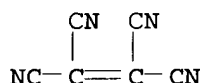
L44 ANSWER 12 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:532353 HCAPLUS
 DOCUMENT NUMBER: 129:276757
 TITLE: A new polyurethane for second-order nonlinear optics

AUTHOR(S): Woo, Han Young; Lee, Kwang-Sup; Shim, Hong-Ku
 CORPORATE SOURCE: Dep. Chem., Korea Advanced Inst. Sci. and Technol., Taejon, 305-791, S. Korea
 SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1998), 39(2), 1095-1096
 CODEN: ACPPAY; ISSN: 0032-3934
 PUBLISHER: American Chemical Society, Division of Polymer Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A new functionalized polyurethane structure with a heteroarom. thiophene ring having a tricyanovinyl group in the polymer side chain was prepared. The mol. weight of the final polymer was determined to be Mn=12,000 and Mw/Mn=2.04. The resulting polymer was soluble in N-methylpyrrolidinone and could be processed into good optical quality films by spin casting at .apprx.100°. The second-order nonlinear coefficient, d33, was determined to be 51 pm/V from measuring the second harmonic generation for a thin polymer film. The outstanding orientational stability of the aligned chromophores was observed up to about 150 C, which originated from the rigid polymer backbone and the stabilizing function of the hydrogen bridges formed between the neighboring polyurethane chains.

IT 670-54-2DP, Tetracyanoethylene, reaction products with polyurethanes
 (preparation and characterization of thiophene- and tricyanovinyl group-containing polyurethanes for second-order nonlinear optics)

RN 670-54-2 HCAPLUS
 CN Ethenetetracarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 37-3 (Plastics Manufacture and Processing)
 Section cross-reference(s): 73

IT 670-54-2DP, Tetracyanoethylene, reaction products with polyurethanes 213741-94-7DP, reaction products with tetracyanoethylene 213741-95-8DP, reaction products with tetracyanoethylene
 (preparation and characterization of thiophene- and tricyanovinyl group-containing polyurethanes for second-order nonlinear optics)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

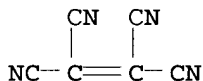
L44 ANSWER 13 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:373193 HCAPLUS
 DOCUMENT NUMBER: 129:68118
 TITLE: Heteroaromatic Chromophore Functionalized Epoxy-Based Nonlinear Optical Polymers
 AUTHOR(S): Wang, Xiaogong; Yang, Ke; Kumar, Jayant; Tripathy, Sukant K.; Chittibabu, Kethinni G.; Li, Lian; Lindsay, Geoffrey
 CORPORATE SOURCE: Center for Advanced Materials Departments of Chemistry and Physics, University of Massachusetts, Lowell, MA, 01854, USA

SOURCE: Macromolecules (1998), 31(13), 4126-4134
 CODEN: MAMOBX; ISSN: 0024-9297
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A series of epoxy-based second-order nonlinear optical (NLO) polymers containing heteroarom. chromophores were designed. Precursor polymers were prepared from diglycidyl ether of Bisphenol A and aniline or 4-(2-thienyl)aniline. The precursor polymers were post-functionalized by an azo-coupling reaction and tricyanovinylolation to form a series of NLO polymers containing heteroarom. chromophores. The versatility of the post-modification strategy previously reported was extended to include various heteroarom. chromophores in the polymers at the final stage of synthesis. The correlation between different heteroarom. chromophore structure and NLO properties of the polymers was extensively studied. Polymers containing heteroarom. chromophores exhibit improved temporal stability and enhanced NLO activity. The d_{33} was 80 pm/V at 1.550 μ m for a representative polymer of the class containing 2-(4-aminophenyl)-(5-tricyanovinyl)thiophene chromophores. The NLO properties of the poled polymers exhibit long-term stability at 80°.

IT 670-54-2DP, Tetracyanoethylene, reaction products with epoxy poly(thienylaniline)s
 (preparation and NLO properties of epoxy-polyaniline and epoxy-polythienylaniline functionalized with heteroarom. chromophores)

RN 670-54-2 HCAPLUS
 CN Ethenetetracarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)

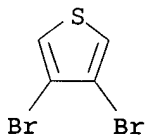


CC 35-8 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 36, 73

IT 121-66-4DP, 2-Amino-5-nitrothiazole, diazonium salts, reaction products with epoxy polyanilines 670-54-2DP, Tetracyanoethylene, reaction products with epoxy poly(thienylaniline)s 6285-57-0DP, 2-Amino-6-nitrobenzothiazole, diazonium salts, reaction products with epoxy polyanilines 30974-11-9DP, Aniline-bisphenol a diglycidyl ether copolymer, reaction products with nitrothiazole and coumarin and cyanoethylene chromophores 39565-05-4DP, 2-Amino-5-(4-nitrophenylsulfonyl)thiazole, diazonium salts, reaction products with epoxy polyanilines 40953-34-2DP, 2-Amino-4,5-imidazoledicarbonitrile, diazonium salts, reaction products with epoxy polyanilines 53518-15-3DP, 7-Amino-4-(trifluoromethyl)coumarin, diazonium salts, reaction products with epoxy polyanilines 208933-69-1DP, Bisphenol A diglycidyl ether-4-(2-thienyl)aniline copolymer, reaction products with nitrothiazole and coumarin and cyanoethylene chromophores
 (preparation and NLO properties of epoxy-polyaniline and epoxy-polythienylaniline functionalized with heteroarom. chromophores)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 14 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:336249 HCAPLUS
DOCUMENT NUMBER: 129:87693
TITLE: Characterizing and circumventing
intermolecular electrostatic interactions in
highly electro-optic polymers
AUTHOR(S): Harper, Aaron W.; Zhu, Jingsong; He, Mingqian;
Dalton, Larry R.; Garner, Sean M.; Steier,
William H.
CORPORATE SOURCE: Departments of Chemistry and of Materials
Science and Engineering, University of
Southern California, Los Angeles, CA,
90089-1661, USA
SOURCE: Materials Research Society Symposium
Proceedings (1998), 488(Electrical, Optical,
and Magnetic Properties of Organic Solid-State
Materials IV), 199-210
CODEN: MRSPDH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In general, polymers possessing nonresonant electrooptic
activities exceeding 20 pm/V require chromophores with strong
electron withdrawing groups (cyanovinyls, C acid moieties, etc.)
as well as highly polarizable bridges. Although much progress was
made on designing and preparing materials with mol. electrooptic
activities, their incorporation into polymers to show comparably
large bulk electrooptic activities was met with little success.
The authors report here the mature of the difficulty of the
translation of microscopic to macroscopic electrooptic activity.
The optimization of mol. activity increases intermol.
electrostatic interactions between chromophores, and these
interactions impede induction of polar acentric order in the
polymers. Theor. anal. of the problem is presented, as well as
one example of a material that is designed to circumvent these
interactions. The resulting material possesses electrooptic
coeffs. ≤ 29 pm/V and optical losses ≥ 1.5 dB/cm.
IT 3141-26-2P
(characterizing and circumventing intermol. electrostatic
interactions in highly electro-optic polymers prepared using)
RN 3141-26-2 HCAPLUS
CN Thiophene, 3,4-dibromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 73-10 (Optical, Electron, and Mass Spectroscopy and
Other Related Properties)
Section cross-reference(s): 36, 38, 77
IT 3141-26-2P 122107-04-4P 151324-67-3P
208389-48-4P 208389-49-5P 208389-50-8P
208389-51-9P 208389-52-0P 208389-53-1P
208389-54-2P 208389-55-3P 208389-56-4P
(characterizing and circumventing intermol. electrostatic

interactions in highly electro-optic polymers prepared using)
 IT 62-75-9, DMNA 2491-74-9 4584-57-0, DANS 189206-46-0
 190438-89-2
 (characterizing and circumventing intermol. electrostatic
 interactions in highly electro-optic polymers prepared using)
 IT 102-71-6, reactions 109-72-8, n-Butyllithium, reactions
 584-84-9 594-19-4, tert-Butyllithium 670-54-2,
 Tetracyanoethylene, reactions 693-04-9, Butyl-magnesium chloride
 3958-03-0, Tetrabromothiophene 7726-95-6, Bromine,
 reactions 7789-60-8, Tribromophosphine 16940-66-2, Sodium
 tetrahydroborate 127278-74-4
 (characterizing and circumventing intermol. electrostatic
 interactions in highly electro-optic polymers prepared using)
 REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L44 ANSWER 15 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:243332 HCAPLUS

DOCUMENT NUMBER: 129:4883

TITLE: Functionalized polyolefinic nonlinear optic
 chromophores incorporating the
 1,3-dithiol-2-ylidene moiety as the
 electron-donating part

AUTHOR(S): Nguyen, T. T.; Salle, M.; Delaunay, J.; Riou,
 A.; Richomme, P.; Raimundo, J. M.; Gorgues,
 A.; Ledoux, I.; Dhenaut, C.; Zyss, J.; Orduna,
 J.; Garin, J.

CORPORATE SOURCE: Lab. Ing. Mol. Mater. Org., UMR CNRS 6501,
 Universite d'Angers, Angers, F-49045, Fr.

SOURCE: Journal of Materials Chemistry (1998), 8(5),
 1185-1192

CODEN: JMACEP; ISSN: 0959-9428

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

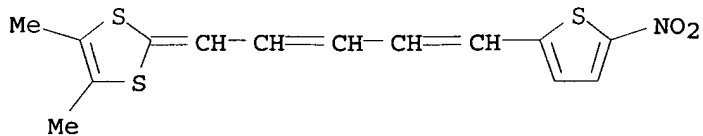
LANGUAGE: English

AB The synthesis of a series of push-pull systems [donor (D)-acceptor
 (A)], associating the 1,3-dithiol-2-ylidene moiety (D) to various (A)
 fragments through polyene linkages of various lengths, is
 described. Design optimization of these NLO phores is via
 systematic determination of the mol. first hyperpolarizabilities (β).
 Selected compds. of this series, displaying the highest β
 values, are then chemical functionalized in order to promote their
 covalent grafting to polymeric backbones.

IT 207510-60-9P
 (preparation of functionalized polyene nonlinear optical
 chromophores incorporating electron-donating
 1,3-dithiol-2-ylidene moiety)

RN 207510-60-9 HCAPLUS

CN 1,3-Dithiole, 4,5-dimethyl-2-[5-(5-nitro-2-thienyl)-2,4-
 pentadienylydene]- (9CI) (CA INDEX NAME)



CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 28, 73

IT 207510-57-4P 207510-58-5P 207510-59-6P 207510-60-9P
207510-62-1P 207510-63-2P 207510-64-3P 207510-65-4P
207510-66-5P 207510-67-6P 207510-68-7P 207510-69-8P
207510-70-1P 207510-71-2P 207510-72-3P 207510-73-4P
207510-74-5P 207510-75-6P 207510-76-7P 207510-77-8P
207510-79-0P 207510-81-4P 207510-83-6P 207510-84-7P
207510-85-8P 207510-87-0P 207510-89-2P 207510-90-5P
207510-91-6P 207510-92-7P 207510-93-8P 207510-94-9P
207510-95-0P 207510-96-1P
(preparation of functionalized polyene nonlinear optical
chromophores incorporating electron-donating
1,3-dithiol-2-ylidene moiety)

IT 98-88-4, Benzoyl chloride 109-77-3, Malononitrile 333-27-7,
Methyl trifluoromethanesulfonate 540-51-2, 2-Bromoethanol
670-54-2, Tetracyanoethylene, reactions 867-13-0,
Triethyl phosphonoacetate 920-46-7, Methacryloyl chloride
2026-42-8, Diethyl (2-thienyl)methylphosphonate
2032-34-0, Cyanoacetaldehyde diethyl acetal 2767-70-6,
4-Nitrobenzyltriphenylphosphonium bromide 4093-49-6,
Fumaraldehyde mono(dimethyl acetal) 10236-14-3, Triethyl
4-phosphonocrotonate 16940-81-1, Hexafluorophosphoric acid
87815-66-5 87815-67-6 128258-71-9 139199-98-7
175393-20-1 207510-55-2 207510-56-3 207510-78-9
(starting material; preparation of functionalized polyene nonlinear
optical chromophores incorporating electron-donating
1,3-dithiol-2-ylidene moiety)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L44 ANSWER 16 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:191945 HCAPLUS

DOCUMENT NUMBER: 128:294725

TITLE: Synthesis of nonlinear optical chromophores
containing electron-excessive and -deficient
heterocyclic bridges. The auxiliary
donor-acceptor effects

AUTHOR(S): Shu, Ching-fong; Wang, Yuh-kai

CORPORATE SOURCE: Department of Applied Chemistry, National
Chiao Tung University, Hsin-Chu, 30035, Taiwan

SOURCE: Journal of Materials Chemistry (1998), 8(4),
833-835
CODEN: JMACEP; ISSN: 0959-9428

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

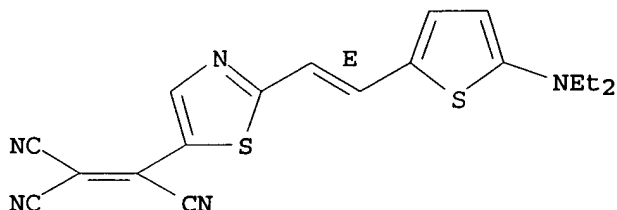
AB Push-pull substituted nonlinear optical chromophores with thiazole
and thiophene rings and interposed ethylene units as
 π -conjugated bridges were synthesized. The effects of the
nature and location of the heterocycles on the energy of the
charge transfer transition for the chromophores are discussed.

IT 206049-78-7P
(preparation of nonlinear optical chromophores containing
electron-excessive and -deficient heterocyclic bridges)

RN 206049-78-7 HCAPLUS

CN Ethenetricarbonitrile, [2-[(1E)-2-[5-(diethylamino)-2-
thienyl]ethenyl]-5-thiazolyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 73
 IT 206049-78-7P 206049-79-8P 206049-80-1P
 206049-81-2P
 (preparation of nonlinear optical chromophores containing
 electron-excessive and -deficient heterocyclic bridges)
 IT 109-77-3, Malononitrile 670-54-2, Tetracyanoethylene,
 reactions 2026-42-8, Diethyl 2-thienylmethylphosphonate
 3034-52-4, 2-Chlorothiazole 3034-53-5, 2-Bromothiazole
 24372-46-1, 5-Diethylamino-2-formylthiophene
 (preparation of nonlinear optical chromophores containing
 electron-excessive and -deficient heterocyclic bridges)
 IT 1005-28-3P, 2-Diethylamino-5-formylthiazole 3364-78-1P,
 2-Chloromethylthiazole 10200-59-6P, 2-Formylthiazole
 14542-12-2P, 2-Hydroxymethylthiazole 115754-94-4P
 206049-74-3P 206049-75-4P 206049-76-5P
 206049-77-6P
 (preparation of nonlinear optical chromophores containing
 electron-excessive and -deficient heterocyclic bridges)
 REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L44 ANSWER 17 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:80159 HCAPLUS
 DOCUMENT NUMBER: 128:186180
 TITLE: Development of functionalized polyetherimides
 for second-order nonlinear optics
 AUTHOR(S): Lee, Kwang-Sup; Moon, Ki-Jeong; Shim, Hong-Ku
 CORPORATE SOURCE: Dep. Macromolecular Sci., Hannam Univ.,
 Taejon, 300-791, S. Korea
 SOURCE: Molecular Crystals and Liquid Crystals Science
 and Technology, Section A: Molecular Crystals
 and Liquid Crystals (1997), 294, 241-244
 CODEN: MCLCE9; ISSN: 1058-725X
 PUBLISHER: Gordon & Breach Science Publishers
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Two types of NLO active linear polyetherimides (PEI-DANS and
 PEI-TH/PEI-TCN) derived from Mitsunobu reaction of diimide and
 hydroxy-functionalized DANS or TCN-type chromophores were prepared
 The TG of the resulting polymers ranged between 144-157°.
 The poled samples were able to produce PEI-DANS and PEI-TH/PEI-TCN
 (23.6% chromophore concentration level) with macroscopic 2nd-order NLO
 activity, $\chi(2)$, values of 73 pm/V and 56 pm/V, resp., at 1063
 nm. In the latter case, no decay of the 2nd harmonic generation
 signal was observed up to 125°. Such excellent thermal
 stability can be attributed to strong chromophore-chromophore

and/or chromophore-polymer backbone interactions.

IT 195058-36-7P
(development of functionalized polyetherimides for second-order nonlinear optics)

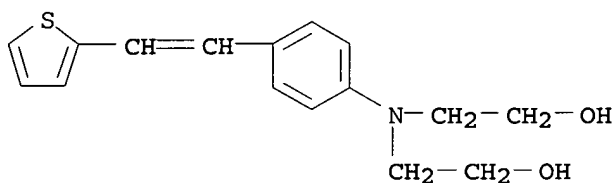
RN 195058-36-7 HCAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis-, polymer with 2,2'-[[4-[2-(2-thienyl)ethenyl]phenyl]imino]bis[ethanol] (9CI) (CA INDEX NAME)

CM 1

CRN 195058-35-6

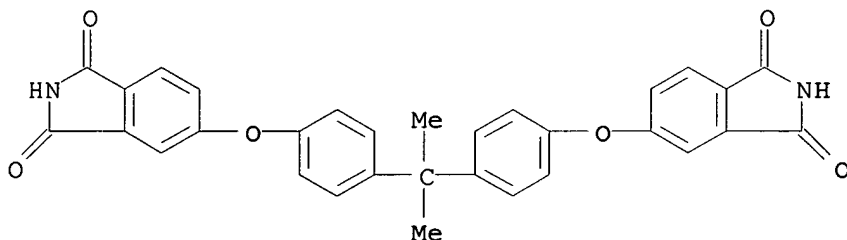
CMF C16 H19 N O2 S



CM 2

CRN 147166-37-8

CMF C31 H22 N2 O6



CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 22

IT 195058-33-4P 195058-34-5P 195058-36-7P
195058-37-8P
(development of functionalized polyetherimides for second-order nonlinear optics)

IT 670-54-2P, Tetracyanoethylene, reactions 117563-47-0P
195058-35-6P
(development of functionalized polyetherimides for second-order nonlinear optics)

IT 603-35-0, Triphenylphosphine, reactions 1080-32-6, Diethyl benzylphosphonate 2026-42-8 19249-34-4 147166-37-8
(development of functionalized polyetherimides for second-order nonlinear optics)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 18 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1997:805546 HCAPLUS
 DOCUMENT NUMBER: 128:35200
 TITLE: Polyamic acids and polyimides with side chains
 conferring or capable of being converted to
 confer nonlinear optical properties, and their
 preparation
 INVENTOR(S): Jen, Kwan Yue Alex; Drost, Kevin Joel
 PATENT ASSIGNEE(S): Enichem S.p.A., Italy
 SOURCE: U.S., 17 pp., Cont.-in-part of U.S. Ser. No.
 132,707, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 5
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5688906	A	19971118	US 1995-500384	1995 0807
US 5514799	A	19960507	US 1993-101368	1993 0802
PRIORITY APPLN. INFO.:			US 1990-626358	B1 1990 1212
			US 1993-101368	A2 1993 0802
			US 1993-132707	B1 1993 1006
			US 1993-158184	A2 1993 1124

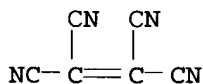
AB A polyamic acid having nonlinear optical (NLO) or pre-NLO side chains is prepared by (1) providing a bis(aromatic dicarboxylic acid anhydride) containing at least one NLO or pre-NLO side chain which contains an electron-donating linking group and an electron-withdrawing moiety or H connected to a π -conjugated noncentrosym. heteroaryl moiety and (2) causing the dianhydride to react with an aromatic diamine; the polyamic acid is converted to the polyimide by standard methods. Alternatively, the diamine or both the dianhydride and the diamine may contain such side chains. In a simpler model system, $\text{PhN}(\text{CH}_2\text{CH}_2\text{OH})_2$ was esterified with 2 mol trimellitic anhydride chloride to give a dianhydride, which was polycondensed with $\text{O}(\text{C}_6\text{H}_4\text{NH}_2\text{-p})_2$ to give a polyamic acid, which was cyclized to the polyimide. The polyimide was treated with $(\text{NC})_2\text{C:C}(\text{CN})_2$ to tricyanovinylate the Ph side groups. Diethanolamine intermediates with heteroaryl substituents were

prepared for use in similar reaction schemes.

IT 670-54-2DP, Tetracyanoethylene, reaction products with polyimides having Ph substituents
(preparation of polyamic acids and polyimides with side chains conferring nonlinear optical properties)

RN 670-54-2 HCAPLUS

CN Ethenetetracarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)



IC C08G069-26; C08G073-10

INCL 528353000

CC 35-5 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 25, 27, 73

IT 670-54-2DP, Tetracyanoethylene, reaction products with polyimides having Ph substituents 155639-81-9DP, reaction products with tetracyanoethylene 155639-82-0DP, reaction products with tetracyanoethylene 163271-35-0P 167268-02-2DP, reaction products with tetracyanoethylene 167268-03-3DP, reaction products with tetracyanoethylene 167268-05-5P
(preparation of polyamic acids and polyimides with side chains conferring nonlinear optical properties)

IT 4182-45-0P, N,N-Bis(2-aminoethyl)aniline 19249-34-4P, Phenylldiethanolamine diacetate 41313-77-3P, 4-[Bis(2-acetoxyethyl)amino]benzaldehyde 99169-09-2P 155639-80-8P 155924-34-8P 167268-04-4P 167268-06-6P
(preparation of polyamic acids and polyimides with side chains conferring nonlinear optical properties)

IT 120-07-0, Phenylldiethanolamine 553-27-5, N,N-Bis(2-chloroethyl)aniline 2026-42-8, Diethyl (2-thienylmethyl)phosphonate 28286-88-6, 4-(Dicyanomethylene)-2,6-dimethyl-4H-pyran
(preparation of polyamic acids and polyimides with side chains conferring nonlinear optical properties)

L44 ANSWER 19 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:528044 HCAPLUS

DOCUMENT NUMBER: 127:234881

TITLE: Highly efficient and thermally stable second-order nonlinear optical polymers

AUTHOR(S): Lee, Kwang Sup

CORPORATE SOURCE: Department Macromolecular Science, Hannam University, Taejon, 300, S. Korea

SOURCE: Macromolecular Symposia (1997), 118, 519-525
CODEN: MSYMEC; ISSN: 1022-1360

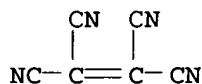
PUBLISHER: Huethig & Wepf

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several functionalized polyurethanes with highly active nonlinear optical chromophores were prepared. The alignment of the chromophores in poled samples exhibited an extended temporal stability due to the hydrogen bonding between the urethane linkage. Thermally stable polyetherimides with an excellent long-term stability of nonlinear activity were also developed. The detailed characterization, including thermal and optical properties, indicated very promising features for photonics

applications of these polymers.
 IT 670-54-2DP, Tetracyanoethylene, reaction products with
 bisphenol A diphthalic anhydride-bis(hydroxyethylamino)phenylethen
 ylthiophene copolymer
 (preparation and second-order nonlinear optical properties of
 polyamide-polyamines)
 RN 670-54-2 HCAPLUS
 CN Ethenetetracarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)



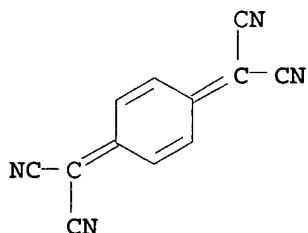
CC 36-5 (Physical Properties of Synthetic High Polymers)
 Section cross-reference(s): 73
 IT 670-54-2DP, Tetracyanoethylene, reaction products with
 bisphenol A diphthalic anhydride-bis(hydroxyethylamino)phenylethen
 ylthiophene copolymer 152100-56-6P 172546-55-3P 172890-15-2P
 186000-81-7P 195058-29-8P 195058-32-3P 195058-33-4P
 195058-34-5P 195058-36-7DP, reaction products with
 tetracyanoethylene 195058-36-7P 195058-37-8DP,
 reaction products with tetracyanoethylene 195058-37-8P
 195159-42-3P
 (preparation and second-order nonlinear optical properties of
 polyamide-polyamines)

L44 ANSWER 20 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:451069 HCAPLUS
 DOCUMENT NUMBER: 127:143456
 TITLE: Tunneling at organic/metal interfaces in
 oligomer-based thin-film transistors
 AUTHOR(S): Garnier, Francis; Kouki, Faycal; Hajlaoui,
 Rhiad; Horowitz, Gilles
 CORPORATE SOURCE: USA
 SOURCE: MRS Bulletin (1997), 22(6), 52-56
 CODEN: MRSBEA; ISSN: 0883-7694
 PUBLISHER: Materials Research Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

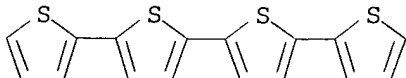
AB The field-effect mobilities in highly pure tetramer and pentamer
 of thiophene are very close to that observed for the hexamer. This
 opens the way for use of shorter and more soluble organic semiconductors
 for applications in solution-processed FETs. The device
 characteristics also can be improved by improving the ohmic
 contact between the organic p-type semiconductor and the metal
 electrode. Surface doping of the organic material, carried out
 through the formation of a charge-transfer complex by use of an
 electron acceptor, e.g. TCNQ, leads to the formation of a p/p+/M
 structure, in which current flow is controlled by field emission.

IT 1518-16-7, TCNQ
 (tunneling at organic/metal interfaces in oligomer-based thin-film
 transistors)
 RN 1518-16-7 HCAPLUS
 CN Propanedinitrile, 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis-
 (9CI) (CA INDEX NAME)



CC 76-3 (Electric Phenomena)
 Section cross-reference(s): 73
 IT 1518-16-7, TCNQ 127473-73-8, Thiophene tetramer
 127473-74-9, Thiophene pentamer
 (tunneling at organic/metal interfaces in oligomer-based thin-film transistors)
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L44 ANSWER 21 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1997:265165 HCAPLUS
 DOCUMENT NUMBER: 126:337334
 TITLE: Improved field-effect mobility in short
 oligothiophenes. Quaterthiophene and
 quinquethiophene
 AUTHOR(S): Hajlaoui, Riadh; Horowitz, Gilles; Garnier,
 Francis; Arce-Bouchet, Alexandre; Laigre,
 Laurent; El Kassmi, Ahmed; Demanze, Frederic;
 Kouki, Faycal
 CORPORATE SOURCE: Laboratoire Materiaux Moleculaires, CNRS,
 Thiais, F-94320, Fr.
 SOURCE: Advanced Materials (Weinheim, Germany) (1997),
 9(5), 389-391
 CODEN: ADVMEW; ISSN: 0935-9648
 PUBLISHER: VCH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Organic field effect transistors made from quaterthiophene (4T) and
 quinquethiophene were fabricated with enhanced field effect
 mobilities. Problems were found rather in achieving efficient
 charge injection than in poor charge transport. In the case of
 4T, the use of a thin layer of tetracyanoquinodimethane as
 electron acceptor between the source and drain Au electrodes and
 the semiconducting layer resulted in an improved mobility, which
 was ascribed to a better carrier injection. Elec. characteristics
 and UV-VIS absorption spectra were shown.
 IT 5632-29-1, Quaterthiophene
 (improved field-effect mobility in quaterthiophene used in organic
 FETs by tetracyanoquinodimethane as electron acceptor)
 RN 5632-29-1 HCAPLUS
 CN 2,2':5',2'':5'',2'''-Quaterthiophene (6CI, 7CI, 8CI, 9CI) (CA
 INDEX NAME)



CC 76-3 (Electric Phenomena)
Section cross-reference(s): 73
IT 5632-29-1, Quaterthiophene
(improved field-effect mobility in quaterthiophene used in organic FETs by tetracyanoquinodimethane as electron acceptor)
IT 5660-45-7
(improved field-effect mobility in quinquethiophene used in organic FETs by tetracyanoquinodimethane as electron acceptor)
IT 1518-16-7, Tetracyanoquinodimethane
(improved field-effect mobility in short oligothiophenes used in organic FETs by tetracyanoquinodimethane as electron acceptor)

L44 ANSWER 22 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:211318 HCAPLUS

DOCUMENT NUMBER: 126:263702

TITLE: An ab Initio and Semiempirical Study of the First- and Third-Order Polarizabilities in Benzene and Thiophene Derivatives: Electron Correlation Effects

AUTHOR(S): Adant, C.; Bredas, J. L.; Dupuis, M.

CORPORATE SOURCE: Service de Chimie des Materiaux Nouveaux
Centre de Recherche en Electronique et Photonique Moleculaires, Universite de Mons-Hainaut, Mons, B-7000, Belg.

SOURCE: Journal of Physical Chemistry A (1997), 101(16), 3025-3031

CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

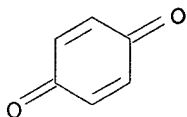
LANGUAGE: English

AB The static first- and third-order polarizabilities of several benzene and thiophene derivs. are evaluated at the ab initio level via an efficacious general finite field approach. The impact of electron correlation is explored by calculating the mol. polarizabilities at the Moller-Plesset second-order perturbation (MP2) theory level using an extended basis set. Further, we examine the influence of mol. architecture on the nonlinear optical response, in particular the switch from an arylethenyl type of structure to a quinoid structure. Finally, we apply the correction vector method combined with the INDO-single and double excitation CI (INDO-SDCI) technique to evaluate the optical nonlinearities at the semiempirical level. The reliability of this procedure is established by comparison with the corresponding high-level ab initio polarizability values. The results clearly show the sensitive dependence of the nonlinear optical properties on electron correlation effects that are found to quant. and qual. affect the third-order polarizability values.

IT 106-51-4, p-Benzoquinone, properties
(ab initio and semiempirical study of structural and electron correlation effects on first- and third-order polarizabilities of benzene and thiophene derivs.)

RN 106-51-4 HCAPLUS

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)

Section cross-reference(s): 73

IT 71-43-2, Benzene, properties 100-42-5, Styrene, properties
 106-51-4, p-Benzoquinone, properties 110-02-1,
 Thiophene 502-86-3, Quinodimethane 1482-91-3,
 1,3,5,7-Octatetraene 1918-82-7, 2-Vinylthiophene
 3249-28-3, 2,4-Hexadienedial 4377-73-5, p-Benzoquinonediimine
 66806-34-6, 2,5-Dihydro-2,5-bis(methylene)thiophene 138846-90-9,
 2,4-Hexadiene-1,6-diimine
 (ab initio and semiempirical study of structural and electron
 correlation effects on first- and third-order polarizabilities
 of benzene and thiophene derivs.)

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L44 ANSWER 23 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:643766 HCAPLUS

DOCUMENT NUMBER: 125:288326

TITLE: Polyquinoline-based nonlinear optical
 materials

INVENTOR(S): Jen, Kwan-Yue Alex; Cai, Yongming

PATENT ASSIGNEE(S): Enichem S.P.A., Italy

SOURCE: Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 729056	A1	19960828	EP 1996-101968	1996 0212
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5679763	A	19971021	US 1995-394382	1995 0224
<--				
AU 9645500	A1	19960905	AU 1996-45500	1996 0214
<--				
AU 696081	B2	19980903		
SG 75763	A1	20001024	SG 1996-2445	1996 0217
<--				
JP 08339001	A2	19961224	JP 1996-38503	

1996
0226

PRIORITY APPLN. INFO.:

US 1995-394382

A

1995
0224

OTHER SOURCE(S): MARPAT 125:288326

AB Compns. exhibiting second-order nonlinear optical properties comprise a noncentrosym. aromatic nonlinear optical compound possessing a delocalized resonance configuration as a guest in a host polyquinoline polymer matrix. The resulting materials are stable at annealing and poling temps., and have good processing characteristics.

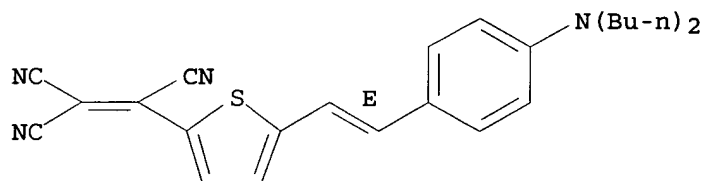
IT 182500-78-3P

(polyquinoline-based hosts containing nonlinear optical materials)

RN 182500-78-3 HCAPLUS

CN Ethenetricarbonitrile, [5-[(1E)-2-[4-(dibutylamino)phenyl]ethenyl]-2-thienyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM G02F001-35

CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 38

IT 182500-78-3P 182500-79-4P

(polyquinoline-based hosts containing nonlinear optical materials)

IT 670-54-2, Tetracyanoethylene, reactions 90134-10-4
182500-77-2

(polyquinoline-based hosts containing nonlinear optical materials)

L44 ANSWER 24 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:631933 HCAPLUS

DOCUMENT NUMBER: 125:288325

TITLE: Process for intramolecularly condensing a non-linear optical polyamic acid composition

INVENTOR(S): Demeuse, Mark T.; Applegate, Diana M.; Jen, Kwan-Yue A.; Kenney, John T.

PATENT ASSIGNEE(S): Enichem S.P.A., Italy

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 727692	A2	19960821	EP 1996-200287	

1996
0208

<--

EP 727692 A3 19960925
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC,
 NL, PT, SE

US 5736592 A 19980407 US 1995-389114

1995
0215

<--

AU 9643364 A1 19960829 AU 1996-43364

1996
0206

<--

AU 703872 B2 19990401
 JP 08269326 A2 19961015 JP 1996-50775

1996
0215

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KR 199865 B1 19990615 KR 1996-3633

1996
0215

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PRIORITY APPLN. INFO.: US 1995-389114 A

1995
0215

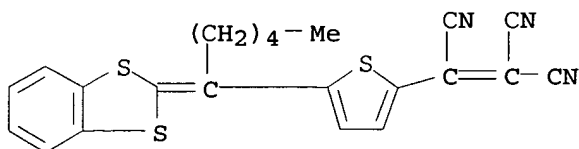
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AB A process for intramolecularly condensing a polyamic acid composition containing a nonlinear optical (NLO) compound to form a polyimide host matrix composition containing as a guest the NLO compound entails uniformly heating the polyamic acid composition, in the absence of a solvent or diluent, to a temperature at which the intramol. condensation will occur without thermal degradation of the NLO compound, so that the temperature differential within the polyamic acid is below that which will produce localized thermal degradation temps., until the intramol. condensation of the polyamic acid composition to the polyimide host matrix composition is substantially complete. Polyimide host matrix comps. containing guest NLO compds. prepared by the inventive process are also disclosed, wherein the NLO compds. have external field-induced mol. alignments.

IT 159968-98-6P
 (methods for intramolecularly condensing nonlinear optical polyamic acid comps.)

RN 159968-98-6 HCAPLUS

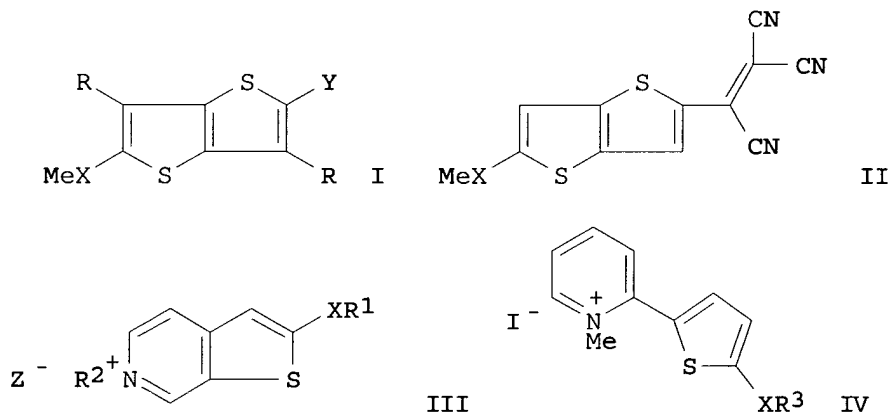
CN Ethenetricarbonitrile, [5-[1-(1,3-benzodithiol-2-ylidene)hexyl]-2-thienyl]- (9CI) (CA INDEX NAME)



IC ICM G02F001-35
 CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
 Section cross-reference(s): 38
 IT 159968-98-6P

(starting material; preparation of nonlinear optical chromophores possessing enhanced thermal stability)

L44 ANSWER 26 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1996:422856 HCAPLUS
 DOCUMENT NUMBER: 125:195463
 TITLE: Chalcogens as electron donors for selected nonlinear optic phores
 AUTHOR(S): Blenkle, Martin; Boldt, Peter; Braeuchle, Christoph; Grahm, Walter; Ledoux, Isabelle; Nerenz, Heiko; Stadler, Stefan; Wichern, Juergen; Zyss, Joseph
 CORPORATE SOURCE: Inst. Organische Chemie, Technische Univ., Braunschweig, D-38092, Germany
 SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1996), (7), 1377-1384
 CODEN: JCPKBH; ISSN: 0300-9580
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

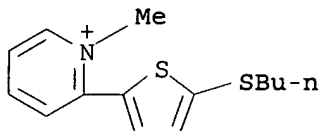


AB Three different heteroarom. charge transfer chromophores, e.g. donor(D)-acceptor(A)-substituted thieno[3,2-b]thiophenes I (R = H, Me; X = O, S, Se; Y = CHO, NO₂) and II (X = O, S, Se, Te), D-substituted thieno[2,3-c]pyridinium salts III (R₁ = C₁₈H₃₇, R₂ = Me, X = S, Z = iodide; R₁ = C₁₈H₃₇, R₂ = Et, X = Se, Z = Br; R₁ = C₁₈H₃₇, R₂ = Me, X = Se, Z = iodide) and 2-(2'-thienyl)pyridinium salts IV (R₃ = Bu, X = S; R₃ = Me, X = Se) have been prepared. Alkylchalcogenic ethers were used as D-groups. The mol. first hyperpolarizabilities β were determined by the EFISH method in the case of I and II and by the HRS method in the case of the ionic compds. III and IV. Substitution of the ether oxygen atom by sulfur increases markedly the β value which is not further increased by the higher chalcogens selenium and tellurium.

IT 180903-99-5P

(preparation and optical properties of thienopyridines, thienylpyridines, and thienothiophenes)

RN 180903-99-5 HCAPLUS
 CN Pyridinium, 2-[5-(butylthio)-2-thienyl]-1-methyl-, iodide (9CI)
 (CA INDEX NAME)



● I⁻

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 29, 73
 IT 180903-86-0P 180903-88-2P 180903-89-3P 180903-90-6P
 180903-91-7P 180903-94-0P 180903-95-1P 180903-96-2P
180903-99-5P 180904-00-1P
 (preparation and optical properties of thienopyridines,
 thienylpyridines, and thienothiophenes)
 IT 112-89-0, 1-Bromooctadecane 251-41-2, Thieno[3,2-b]thiophene
 272-12-8, Thieno[2,3-c]pyridine 542-69-8, 1-Iodobutane
 629-45-8, Dibutyl disulfide **670-54-2**,
 Tetracyanoethylene, reactions 2500-88-1, Dioctadecyl disulfide
3319-99-1 40985-54-4 56412-11-4 56412-12-5
 56412-24-9
 (preparation and optical properties of thienopyridines,
 thienylpyridines, and thienothiophenes)
 IT 180903-81-5P 180903-82-6P 180903-84-8P 180903-92-8P
 180903-93-9P **180903-97-3P 180903-98-4P**
 (preparation and optical properties of thienopyridines,
 thienylpyridines, and thienothiophenes)

L44 ANSWER 27 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1995:780291 HCAPLUS
 DOCUMENT NUMBER: 123:183001
 TITLE: Tricyanovinyl substitution process for
 nonlinear optical polymers
 INVENTOR(S): Drost, Kevin J.; Varanasi, Pushkara R.; Jen,
 Kwan-Yue A.; Drzewinski, Michael A.
 PATENT ASSIGNEE(S): Enichem S.p.A., Italy
 SOURCE: U.S., 22 pp. Cont.-in-part of U.S. Ser. No.
 626,358, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: **Patent**
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 5
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 5395556	A	19950307	US 1991-773708	1991 1009

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CA 2057402 AA 19920613 CA 1991-2057402 1991
1211

EP 493716 A1 19920708 EP 1991-121269 <--
1991
1211

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE <--
JP 06157511 A2 19940603 JP 1991-360918 1991
1212

PRIORITY APPLN. INFO.: US 1990-626358 B2 <--
1990
1212

US 1991-773708 A <--
1991
1009

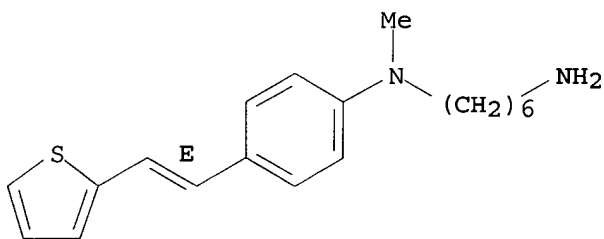
AB Methods of preparing a polymer having second order nonlinear optical properties by reacting the base polymers of the present invention with tetracyanoethylene in a basic solvent at elevated temps. are described. Base polymers devoid of nonlinear optical properties exhibit second order nonlinear optical properties after the covalent attachment of tricyanovinyl groups to pendant side chains of the base polymer.

IT 146823-54-3DP, reaction products with maleic anhydride-styrene copolymers (tricyanovinyl substitution processes for nonlinear optical polymer preparation)

RN 146823-54-3 HCAPLUS

CN 1,6-Hexanediamine, N-methyl-N-[4-[2-(2-thienyl)ethenyl]phenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM F21V009-00
ICS C08G059-00; C08G073-06

INCL 252582000

CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 38

IT 9011-13-6DP, Maleic anhydride-styrene copolymer, imidated, reaction products with thiophene derivs. and tetracyanoethylene 146823-54-3DP, reaction products with maleic anhydride-styrene copolymers 167407-14-9DP, reaction products with tetracyanoethylene 167407-15-0DP, reaction

products with tetracyanoethylene 167407-18-3DP, reaction
products with maleic anhydride-styrene copolymers
(tricyanovinyl substitution processes for nonlinear optical
polymer preparation)

IT 167407-13-8P 167407-14-9P 167407-15-0P

(tricyanovinyl substitution processes for nonlinear optical
polymer preparation)

IT 167407-12-7P

(tricyanovinyl substitution processes for nonlinear optical
polymer preparation)

IT 68-12-2, reactions 100-61-8, N-Methylaniline, reactions
103-76-4, 1-(2-Hydroxyethyl) piperazine 108-24-7, Acetic
anhydride 121-44-8, Triethylamine, reactions 122-52-1,
Triethylphosphite 636-72-6, 2-Hydroxymethyl thiophene
670-54-2, Tetracyanoethylene, reactions 920-46-7,
Methacryloyl chloride 2009-83-8, 6-Chlorohexanol 7719-09-7,
Thionyl chloride 7774-74-5, Thiophene-2-thiol
10025-87-3, Phosphoric trichloride

(tricyanovinyl substitution processes for nonlinear optical
polymer preparation)

IT 765-50-4P, 2-Chloromethyl thiophene 2026-42-8P

120654-22-0P 120654-36-6P, N-(6-Hydroxyhexyl)-N-methylaniline

120654-37-7P, N-(6-Acetoxyhexyl)-n-methylaniline

146823-48-5P 146823-49-6P 146823-50-9P

146823-51-0P 146823-52-1P 146823-53-2P

146823-54-3P 146823-55-4P 146823-56-5P

146823-57-6P 167407-16-1P 167407-17-2P

167407-18-3P

(tricyanovinyl substitution processes for nonlinear optical
polymer preparation)

L44 ANSWER 28 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:695700 HCAPLUS

DOCUMENT NUMBER: 123:182657

TITLE: Tg effects in highly efficient, second order
nonlinear optical side chain polymers

AUTHOR(S): Drost, K. J.; Jen, K. Y.; Drzewinski, M. A.

CORPORATE SOURCE: EniChem America, Inc., Monmouth Junction, NJ,
08852, USA

SOURCE: Polymer Preprints (American Chemical Society,
Division of Polymer Chemistry) (1994), 35(2),
252-3

CODEN: ACPPAY; ISSN: 0032-3934

PUBLISHER: American Chemical Society, Division of Polymer
Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

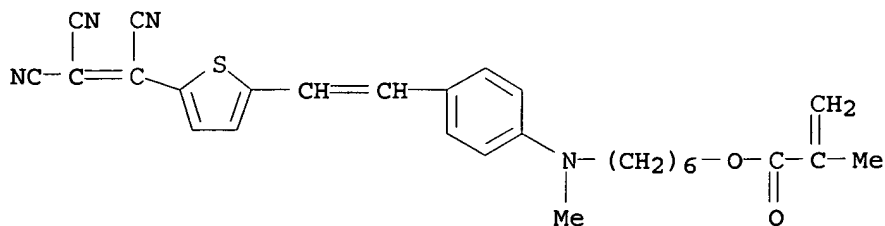
AB A synthetic method was developed to produce high incorporation of
efficient 2nd order nonlinear optical (NLO) chromophores in
styrene and Me methacrylate based polymers. The method involves a
2 step reaction by which the final optical properties are achieved
by reaction of a nonactive precursor polymer. Interesting
variations in Tg with NLO incorporation are seen in the nonactive
state materials vs. the final optically active state. This
behavior is explained by consideration of the high dipole moment
present in the final polymers.

IT 147041-48-3

(formation and attempted polymerization in attempted preparation of
nonlinear optical side chain polymers)

RN 147041-48-3 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, 6-[methyl[4-[2-[5-(tricyanoethenyl)-2-thienyl]ethenyl]phenyl]amino]hexyl ester (9CI) (CA INDEX NAME)



CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 35, 36

IT 147041-48-3
(formation and attempted polymerization in attempted preparation of nonlinear optical side chain polymers)

IT 167497-28-1 167497-30-5
(formation and reaction in preparation of nonlinear optical side chain polymers)

IT 154506-50-0
(formation and reaction with TCNE in preparation of nonlinear optical side chain polymers)

IT 167497-26-9
(formation and reaction with TCNE or Me methacrylate in preparation of nonlinear optical side chain polymers)

IT 167497-25-8 167497-26-9
(formation and reaction with methacroyl chloride in preparation of nonlinear optical side chain polymers)

IT 147041-49-4P 147041-51-8P
(preparation and nonlinear optical properties of)

IT 78-67-1, AIBN 80-62-6 670-54-2,
Ethenetetracarbonitrile, reactions 920-46-7 2026-42-8
9011-13-6 167497-23-6 167497-24-7
(reaction in preparation of nonlinear optical side chain polymers)

L44 ANSWER 29 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:683906 HCAPLUS

DOCUMENT NUMBER: 123:258441

TITLE: Optical and electrical properties of doped poly-3-octylthiophene films

AUTHOR(S): Lidberg, Russell L.; Goswami, Kisholoy; Lovato, Marvin R.; Venkatasubramanian, R.; Engelmann, William H.

CORPORATE SOURCE: Harry Reid Center Environmental Studies, University Nevada, Las Vegas, NV, 89154-4009, USA

SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1995), 2397(Optoelectronic Integrated Circuit Materials, Physics, and Devices), 633-42
CODEN: PSISDG; ISSN: 0277-786X

PUBLISHER: SPIE-The International Society for Optical Engineering

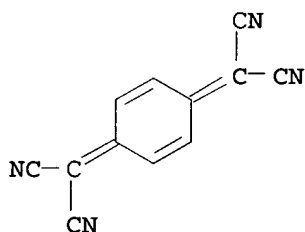
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Optical absorption and elec. conductivity of solution-doped

poly(3-octylthiophene) (P3OT) films were studied. Chloroform solns. of P3OT were doped with the inorg. electron acceptor ferric chloride (FeCl₃) and either 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) or 7,7,8,8-tetracyanoquinodimethane (TCNQ). Charge transfer was observed in P3OT solns. doped with FeCl₃ and DDQ. TCNQ-doped solns. showed no optical evidence of charge transfer. Thin films of the doped P3OT were examined at various doping levels. Spectroscopic and elec. conductivity measurements of P3OT films, doped with DDQ, TCNQ, and FeCl₃ at different doping levels are presented. Optical absorption provided information on the degree of charge transfer occurring for the various dopants. Elec. conductivity measurements showed that the conductivity of P3OT increased with the various dopants in the order of TCNQ < DDQ < FeCl₃ for the same dopant level. Results are discussed in relation to the electrochem. properties of the prepared films.

IT 1518-16-7
(optical and elec. properties of doped poly(3-octylthiophene) films)
RN 1518-16-7 HCAPLUS
CN Propanedinitrile, 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis-
(9CI) (CA INDEX NAME)



CC 37-5 (Plastics Manufacture and Processing)
Section cross-reference(s): 73, 76
IT 84-58-2, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone
1518-16-7 7705-08-0, Ferric chloride, properties
(optical and elec. properties of doped poly(3-octylthiophene) films)
IT 104934-51-2, Poly(3-octylthiophene)
(optical and elec. properties of doped poly(3-octylthiophene) films)

L44 ANSWER 30 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:654956 HCAPLUS
DOCUMENT NUMBER: 123:156088
TITLE: 1,1-vinyl substituted nonlinear optical materials
INVENTOR(S): Varanasi, Pushkara Rao; Jen, Kwan-Yue Alex; Wong, King Young; Mininni, Robert Mark
PATENT ASSIGNEE(S): Enichem S.p.A., Italy
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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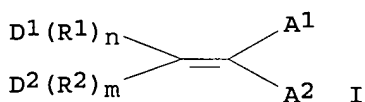
 EP 637774 A1 19950208 EP 1994-111990
1994
0801

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 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL,
 PT, SE
 US 5514799 A 19960507 US 1993-101368
1993
0802

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 JP 07173116 A2 19950711 JP 1994-227195
1994
0802

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 PRIORITY APPLN. INFO.: US 1993-101368 A
1993
0802

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 OTHER SOURCE(S): MARPAT 123:156088
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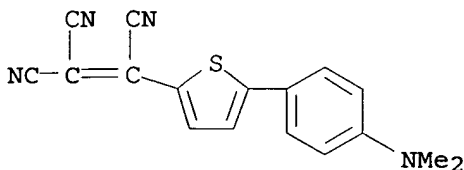
AB Nonlinear optical compds. are described by the general formula I (A1 and A2 are independently selected electron-withdrawing moieties; R1 and R2 are independently selected from aromatic rings, heteroarom. rings and fused ring systems consisting of two or three aromatic or heteroarom. rings; n and m are integers from 1-5; and D1 and D2 are independently selected from hydrogen, electron donating groups and polymer attachment groups, with the restriction that at least one of D1 and D2 is an electron-donating group). Polymers blended with, cured with, or having pendant side chains of the disclosed nonlinear optical materials and exhibiting second order nonlinear properties are also disclosed.

IT **164462-69-5P**

(vinyl substituted nonlinear optical materials)

RN 164462-69-5 HCAPLUS

CN Ethenetricarbonitrile, [5-[4-(dimethylamino)phenyl]-2-thienyl]-
 (9CI) (CA INDEX NAME)



IC ICM G02F001-35

CC 73-10 (Optical, Electron, and Mass Spectroscopy and

Other Related Properties)

Section cross-reference(s): 23

- IT 129437-36-1P 164462-69-5P
(vinyl substituted nonlinear optical materials)
- IT 85299-19-0P 164462-66-2P 164462-70-8P
164516-22-7P
(vinyl substituted nonlinear optical materials)
- IT 110-02-1, Thiophene 110-18-9 142-61-0, Hexanoyl
chloride 492-97-7, 2,2'-Bithiophene 591-51-5,
Phenyllithium 606-23-5, 1H-Indene-1,3(2H)-dione 670-54-2
, Tetracyanoethylene, reactions 1197-19-9, 4-
(Dimethylamino)benzonitrile 1226-46-6, 4,4'-
Bis(dimethylamino)thiobenzophenone 4096-21-3,
1-Phenylpyrrolidine 5217-47-0, 1,3-Diethyl-2-thiobarbituric acid
13411-42-2, 2-Trimethylsilyl-1,3-dithiane 19983-18-7
62217-21-4 88613-62-1
(vinyl substituted nonlinear optical materials)
- IT 26447-67-6P, 2-Hexanoylthiophene 159968-84-0P
164462-67-3P
(vinyl substituted nonlinear optical materials)
- IT 164462-68-4P 164462-71-9P 164462-73-1P
164462-74-2P 164516-21-6P
(vinyl substituted nonlinear optical materials)

L44 ANSWER 31 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:478064 HCAPLUS

DOCUMENT NUMBER: 122:214800

TITLE: Functionalized aromatic heterocyclic compounds
for nonlinear optical materialsINVENTOR(S): Jen, Kwang Yue A.; Varanasi, Pushkara R.;
Drost, Kevin J.; Wong, King Y.

PATENT ASSIGNEE(S): Enichem S.p.A., Italy

SOURCE: Can. Pat. Appl., 60 pp.

CODEN: CPXXEB

DOCUMENT TYPE: Patent

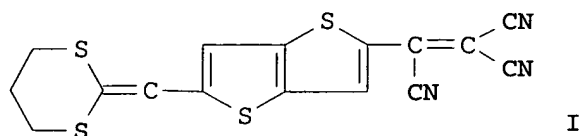
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2104038	AA	19940215	CA 1993-2104038	1993 0813
EP 585999	A1	19940309	EP 1993-202330	1993 0807
JP 06211868	A2	19940802	JP 1993-202387	1993 0816
PRIORITY APPLN. INFO.:				US 1992-930732 A

OTHER SOURCE(S): MARPAT 122:214800
GI



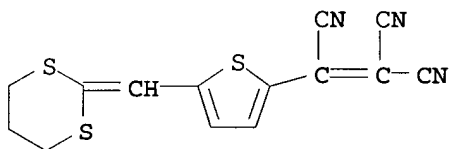
AB Compds. showing nonlinear optical properties (second-harmonic generation), e.g., 2-(1,3-dithian-2-ylidenemethyl)-5-(tricyanovinyl)thieno[3,2-b]thiophene (I) or 2-(1,3-dithian-2-ylidenemethyl)-5-(tricyanovinyl)thiophene, are prepared. The compds. are useful in the preparation of polymers showing nonlinear optical properties. Reacting 2-formylthieno[3,2-b]thiophene with 2-trimethylsilyl-1,3-dithiane and tricyanoethylene gave I.

IT 157841-21-9P

(preparation and nonlinear optical properties of)

RN 157841-21-9 HCAPLUS

CN Ethenetricarbonitrile, [5-(1,3-dithian-2-ylidenemethyl)-2-thienyl]-(9CI) (CA INDEX NAME)



IC ICM C07D495-14

ICS C07D495-04; C07D493-12; C07D487-14; C07D517-14; C07D409-00;
C07F009-547; C08F008-50; C08G083-00

CC 35-1 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 28, 36, 37, 73

IT 157841-21-9P 159120-91-9P 159120-92-0P

160247-48-3P 160247-49-4P 160247-50-7P

162124-83-6P 162124-84-7P 162124-85-8P 162124-90-5P

(preparation and nonlinear optical properties of)

IT 162124-92-7P 162124-93-8P 162124-94-9P

162124-95-0P 162124-96-1P 162124-97-2P 162124-98-3P

(preparation and reaction with tetracyanoethylene)

IT 98-03-3, 2-Formylthiophene

(reaction with dithiane derivs.)

IT 670-54-2, Tetracyanoethylene, reactions

(tricyanovinylolation of thiophene derivs. by)

L44 ANSWER 32 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:272889 HCAPLUS

DOCUMENT NUMBER: 122:67889

TITLE: Efficient electron-donating groups for
nonlinear optical applications

INVENTOR(S): Jen, Kwan Yue Alex; Drost, Kevin Joel; Wong,
King Young; Varanasi, Pushkara Rao; Mininni,
Robert Mark

PATENT ASSIGNEE(S): Enichem S.p.A., Italy

SOURCE: Eur. Pat. Appl., 26 pp.

DOCUMENT TYPE: CODEN: EPXXDW
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: English
 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 602654	A1	19940622	EP 1993-120340	1993 1216

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC,
 NL, PT, SE

JP 06228153	A2	19940816	JP 1993-343245	1993 1217
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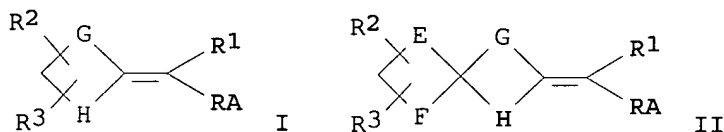
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PRIORITY APPLN. INFO.: US 1992-992625 A

1992
1218

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OTHER SOURCE(S): MARPAT 122:67889
 GI



AB Nonlinear optical materials having structures with delocalized resonance configurations corresponding are described by the general formulas I and II (A is a first electron accepting group; R is a pi-conjugated non-centrosym. organic moiety; R2 and R3 are independently selected from hydrogen, alkyl moieties and functionalized alkyl moieties; E, F, G and H are members of a saturated or unsatd. five- to ten-membered cyclic ring or two-ring systems having five- to ten-membered rings that are electron donating in nature and E, F, G and H are independently selected from -CH-, -CH2-, O, S, N, Se, Te, and -NR4-; R4 is selected from hydrogen, alkyl moieties and functionalized alkyl moieties; and R1 is selected from alkyl moieties and functionalized alkyl moieties). Polymers blended with or having the disclosed nonlinear optical materials as pendant side chains and exhibiting second order nonlinear optical properties are also disclosed.

IT 110-02-1, Thiophene
 (efficient electron-donating groups for nonlinear optical applications)

RN 110-02-1 HCAPLUS

CN Thiophene (8CI, 9CI) (CA INDEX NAME)



IC ICM G02F001-35
ICS C07D409-06; C07D409-14; C07D417-06; C07D495-04

CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 27, 28

IT 75-36-5, Acetyl chloride 109-77-3, Malononitrile 110-02-1, Thiophene 142-61-0, Hexanoyl chloride 251-41-2, Thieno[3,2-b]thiophene 492-97-7, 2,2'-Bisthiophene 670-54-2, Tetracyanoethylene, reactions 764-85-2, Nonanoyl chloride 932-16-1, 2-Acetyl N-methyl pyrrole 1192-62-7, 2-Acetyl furan 5217-47-0, 1,3-Diethyl-2-thiobarbituric acid 13218-13-8, Nitroacetonitrile 24295-03-2, 2-Acetyl thiazole 38172-19-9 62217-21-4 111744-23-1, Terthiophene 122301-25-1 133165-45-4 159969-07-0
(efficient electron-donating groups for nonlinear optical applications)

IT 88-15-3P, 2-Acetylthiophene 26447-67-6P, 2-Hexanoyl thiophene 159968-83-9P 159968-84-0P 159968-85-1P 159968-86-2P 159968-87-3P 159968-88-4P 159968-89-5P 159968-90-8P 159968-91-9P 159968-92-0P 159969-06-9P 159969-08-1P 159969-09-2P 159969-10-5P 159969-11-6P 159969-12-7P
(efficient electron-donating groups for nonlinear optical applications)

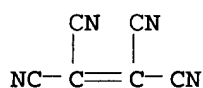
IT 3515-18-2P 159968-93-1P 159968-94-2P 159968-95-3P 159968-96-4P 159968-97-5P 159968-98-6P 159968-99-7P 159969-00-3P 159969-01-4P 159969-02-5P 159969-03-6P 159969-04-7P 159969-05-8P 159969-13-8P 159969-14-9P 159969-15-0P 159969-16-1P
(efficient electron-donating groups for nonlinear optical applications)

L44 ANSWER 33 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:254267 HCAPLUS
DOCUMENT NUMBER: 122:91597
TITLE: Electron and energy transfer processes of photoexcited oligothiophenes onto tetracyanoethylene and C60
AUTHOR(S): Janssen, R. A. J.; Moses, D.; Sariciftci, N. S.
CORPORATE SOURCE: Institute Polymers Organic Solids, University California, Santa Barbara, CA, 93106, USA
SOURCE: Journal of Chemical Physics (1994), 101(11), 9519-27
CODEN: JCPSA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors present near-steady-state photoinduced absorption (PIA) studies on photoexcited states of oligothiophenes (nT, n = 6,7,9,11) in solution Photoexcitation in solution reveals efficient formation of a metastable triplet state (3nT). Oligothiophene

radical cations (nT+) are formed from the singlet excited state via electron transfer to the medium in solvents of high electron affinity. The reactivity of the 3nT state towards acceptor mols. was studied. In the presence of C60 an energy transfer reaction is observed which quenches the 3nT state and produces 3C60 via photosensitization. Addition of tetracyanoethylene (TCNE) results in quenching of the 3nT state via electron transfer and efficiently produces the corresponding nT+ radical cations, as evidenced from PIA and light-induced ESR.

IT 670-54-2, Tetracyanoethylene, miscellaneous
(electron and energy transfer processes of photoexcited oligothiophenes onto tetracyanoethylene and fullerene C60)
RN 670-54-2 HCAPLUS
CN Ethenetetracarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 73-1 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
IT 670-54-2, Tetracyanoethylene, miscellaneous 99685-96-8, Fullerene c60
(electron and energy transfer processes of photoexcited oligothiophenes onto tetracyanoethylene and fullerene C60)
IT 134682-70-5 136313-35-4 136313-40-1
157411-34-2 160466-24-0 160637-37-6
160637-38-7 160638-09-5
(electron and energy transfer processes of photoexcited oligothiophenes onto tetracyanoethylene and fullerene C60)

L44 ANSWER 34 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:245976 HCAPLUS

DOCUMENT NUMBER: 120:245976

TITLE: A new synthetic approach for the incorporation of highly efficient second-order nonlinear optical chromophores containing tricyanovinyl electron acceptors into methacrylate polymers
AUTHOR(S): Dorst, Kevin J.; Rao, V. Pushkara; Jen, Alex K. Y.

CORPORATE SOURCE: Res. Dev. Cent., EniChem America Inc., Monmouth Junction, NJ, 08852, USA

SOURCE: Journal of the Chemical Society, Chemical Communications (1994), (4), 369-71
CODEN: JCCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

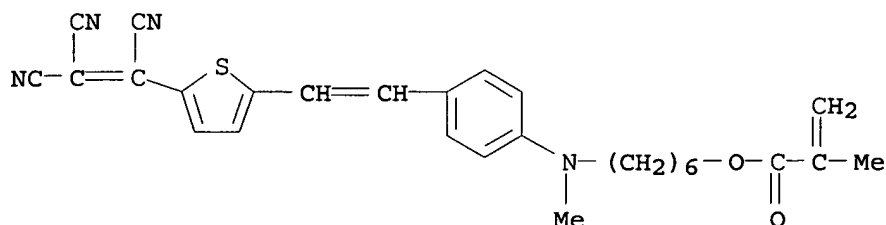
LANGUAGE: English

AB A new synthetic method is developed to incorporate efficient nonlinear optical chromophores containing thiophene conjugating units and tricyanovinyl acceptors into methacrylate polymers. This approach emphasizes the incorporation of tricyanovinyl groups into the pendant side chains after copolymn. of the precursor substituted acrylates with Me methacrylate.

IT 147041-48-3P
(preparation and attempted polymerization of)

RN 147041-48-3 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, 6-[methyl[4-[2-[5-(tricyanoethenyl)-2-thienyl]ethenyl]phenyl]amino]hexyl ester (9CI) (CA INDEX NAME)



- CC 35-8 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 73
- IT 147041-48-3P
(preparation and attempted polymerization of)
- IT 670-54-2DP, Tetracyanoethylene, reaction products with Me methacrylate-[methyl(thienylvinyl)anilino]hexyl methacrylate copolymer 154506-50-0DP, tricyanovinylated
(preparation and nonlinear optical properties of)
- IT 154506-49-7P
(preparation and polymerization of, with Me methacrylate)
- IT 154506-50-0P
(preparation and properties and reaction of, with tetracyanoethylene)
- IT 154506-48-6P
(preparation and reaction of, with methacryloyl chloride)
- IT 2026-42-8, Diethyl 2-thienylphosphonate
(reaction of, with [(acetoxihexyl)methylamino]benzaldehyde)
- IT 670-54-2, Tetracyanoethylene, reactions
(reaction of, with [methyl(thienylvinyl)anilino]hexyl methacrylate)

L44 ANSWER 35 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:417259 HCAPLUS

DOCUMENT NUMBER: 119:17259

TITLE: Competitive bimolecular electron- and energy-transfer quenching of the excited state(s) of the tetranuclear copper(I) cluster Cu₄I₄py₄. Evidence for large reorganization energies in an excited-state electron transfer

AUTHOR(S): Dossing, Anders; Ryu, Chong Kul; Kudo, Setsuko; Ford, Peter C.

CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, 93106, USA

SOURCE: Journal of the American Chemical Society (1993), 115(12), 5132-7

CODEN: JACSAT; ISSN: 0002-7863

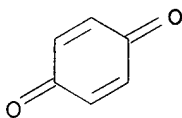
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The quenching of emission from the cluster-centered (ds/XMCT) excited state of the copper(I) cluster Cu₄I₄py₄ (I, py = pyridine) by tris(β-dionato)chromium(III) complexes CrL₃ and several organic substrates was investigated in dichloromethane solution. The E₀₀ energy of the excited state (I*) was estimated to be 1.66 μm⁻¹ (2.06 V), and the reduction potential E_{1/2}(I*/I*) was estimated as -1.78 V (vs the ferrocenium/ferrocene couple). Each of the CrL₃ complexes (2Eg .apprx. 1.3 μM⁻¹) is capable of energy transfer quenching, and the rate of this process is shown to be about 10⁷, 9 M⁻¹s⁻¹. Contributions to the quenching by an apparent electron-transfer

mechanism were evident for those substrates with reduction potentials $E_{1/2}(Q/Q^-)$ less than 1.4 V, i.e. reaction driving forces $(-\Delta G^\circ)$ greater than p.4 V. The large driving force required can be attributed to a very slow I/I^* self-exchange rate and is indicative of large contributions from inner sphere terms to the total electron-transfer reorganization energy. Such contributions are a likely explanation of the substantially pos. ΔH_q .dbldag. values (up to +40 kJ mol⁻¹) noted for organic quenchers with $E_{1/2}(Q/Q^-)$ near 1.4 V. Pressure effect studies demonstrate that the activation volume (ΔV_q .dbldag.) for energy-transfer quenching of the CrL3 species is .apprx.0 cm³ mL⁻¹ while that of those quenchers which operate near the diffusion limit is .apprx.»7 cm³mol⁻¹, consistent with the expected effects on solvent viscosity. In contrast, for those systems with $E_{1/2}(Q/Q^-)$.apprx. 1.4 V, substantially neg. ΔV_q .dbldag. values were observed, a feature reflective of the solvent reorganization owing to charge creation upon electron transfer between I^* and Q.

IT 106-51-4, 1,4-Benzoquinone, properties
(quenching of emission from copper-iodo-pyridine complex by)
RN 106-51-4 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
IT Luminescence quenching
(of copper-iodo-pyridine complex, by chromium dionato complexes and organic compds.)
IT 99-65-0, m-Dinitrobenzene 100-25-4, p-Dinitrobenzene
106-51-4, 1,4-Benzoquinone, properties 528-29-0,
o-Dinitrobenzene 13938-89-1 14592-80-4 14592-89-3
15025-13-5 15488-08-1 21102-39-6 21679-31-2,
Chromium tris(acetylacetonate) 21679-35-6 28096-65-3
(quenching of emission from copper-iodo-pyridine complex by)

L44 ANSWER 36 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:580151 HCAPLUS

DOCUMENT NUMBER: 113:180151

TITLE: Electrochemical and optical characterization of poly(3-methylthiophene). Effects of solvent, anion, and applied potential

AUTHOR(S): Pern, Fu Jann; Frank, Arthur J.

CORPORATE SOURCE: Sol. Energy Res. Inst., Golden, CO, 80401, USA

SOURCE: Journal of the Electrochemical Society (1990), 137(9), 2769-77

CODEN: JESOAN; ISSN: 0013-4651

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electrochem. and optical properties poly(3-methylthiophene) (PMeT) coatings on electrodes exposed to different electrolytes, solvents, redox species, and applied potential were investigated. Electroanal. (cyclic voltammetry, chronoamperometry, chronocoulometry electrode admittance) and spectrophotometric

measurements show that the nature of the charge-compensating dopant anion, the solvent (acetonitrile vs. water), and the applied potential have a profound effect on charge transport through the film. The oxidation (doping) of PMeT films, in contrast to its reduction (undoping), depends on the size of the dopants (BF₄⁻, ClO₄⁻, PF₆⁻, and CF₃SO₃⁻). The film suffers irreversible loss of electrochem. activity, to varying degrees, in aqueous solns. with ions, such as PO₄³⁻, SO₄²⁻, CH₃COO⁻, and phthalate. Ion trapping and slow structural relaxation in the polymeric films introduce hysteresis in the electrochem. and optical data. The doping of the film and the structural relaxation time, associated with its oxidation and reduction, depend strongly on the solvent. The electrochem. activity of PMeT films, in the electronic insulative state, is found to display an unusual dependence on the solvent and the applied potential. The nature of the polymer-dopant and polymer-solvent interactions and the mechanism of charge transport in PMeT are discussed.

IT 84928-92-7, Poly(3-methylthiophene)
(electrochem. and optical characterization of, anions and solvent and potential effect on)

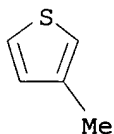
RN 84928-92-7 HCAPLUS

CN Thiophene, 3-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 616-44-4

CMF C5 H6 S



CC 72-2 (Electrochemistry)

Section cross-reference(s): 36, 73

IT 84928-92-7, Poly(3-methylthiophene)
(electrochem. and optical characterization of, anions and solvent and potential effect on)

IT 616-44-4, 3-Methylthiophene
(polymerization of, electrochem., conducting polymer from, anion effect on)

IT 1518-16-7, TCNQ 13408-63-4, Ferrocyanide 13601-18-8
15305-72-3
(redox reaction of, on electrodes with poly(methylthiophene))

L44 ANSWER 37 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:607880 HCAPLUS

DOCUMENT NUMBER: 107:207880

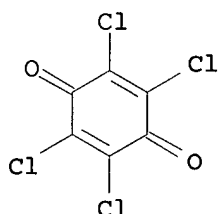
TITLE: Extinction coefficients of triplet-triplet absorption spectra of organic molecules in condensed phases: a least-squares analysis

AUTHOR(S): Carmichael, Ian; Helman, W. P.; Hug, G. L.
CORPORATE SOURCE: Radiat. Chem. Data Cent., Univ. Notre Dame, Notre Dame, IN, 46556, USA

SOURCE: Journal of Physical and Chemical Reference Data (1987), 16(2), 239-60
CODEN: JPCRBU; ISSN: 0047-2689

DOCUMENT TYPE: Journal
 LANGUAGE: English

- AB A global least-squares technique was developed to assist in the critical evaluation of data consisting of large sets of measurements. The technique was designed to handle sets of data where many of the measurements are relative measurements. A linearization procedure was used to reduce the inherently nonlinear problem to a traditional multivariate linear regression. The technique was used to evaluate extinction coeffs., ϵ 's, of triplet-triplet absorption (TTA) spectra of organic mols. in condensed phases. A previous assumption, that there are no solvent effects on the TTA spectra, was investigated and modified so that a group of compds. measured in PhH was treated sep. The set of 445 ϵ 's obtained from the global least-squares fit, including these solvent effects, are presented. How these least-squares results can be used in a hierarchy of TTA ϵ stds. is discussed. Further solvent effects such as the separation of polar and nonpolar media and the influence of temperature were probed.
- IT 118-75-2, Chloranil, properties
 (extinction coefficient of, global least-squares fit of)
- RN 118-75-2 HCAPLUS
- CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro- (9CI) (CA INDEX NAME)



- CC 73-4 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
 Section cross-reference(s): 22
- IT 50-89-5, Thymidine, properties 53-70-3, Dibenz[a,h]anthracene
 54-12-6 56-55-3, Benz[a]anthracene 57-87-4, Ergosterol
 58-27-5, 2-Methyl-1,4-naphthoquinone 58-96-8, Uridine 58-97-9,
 Uridine monophosphate, properties 65-71-4, Thymine 65-85-0,
 Benzoic acid, properties 65-86-1, Orotic acid 66-22-8,
 properties 66-97-7, Psoralen 67-64-1, Acetone, properties
 68-26-8 71-43-2, properties 73-22-3, properties 73-97-2,
 Orotate ion 74-31-7, N,N'-Diphenyl-p-phenylenediamine 79-77-6,
 β -Ionone 82-45-1, 1-Aminoanthraquinone 83-32-9,
 Acenaphthene 85-01-8, Phenanthrene, properties 86-28-2,
 N-Ethylcarbazole 86-73-7, Fluorene 86-74-8, Carbazole
 90-11-9, 1-Bromonaphthalene 90-12-0, 1-Methylnaphthalene
 90-13-1, 1-Chloronaphthalene 90-44-8, Anthrone 90-47-1,
 Xanthone 90-96-0, 4,4'-Dimethoxybenzophenone 90-98-2,
 4,4'-Dichlorobenzophenone 91-20-3, Naphthalene, properties
 91-22-5, Quinoline, properties 91-44-1, 7-Diethylamino-4-
 methylcoumarin 91-57-6, 2-Methylnaphthalene 91-64-5, Coumarin
 92-06-8, m-Terphenyl 92-24-0, Tetracene 92-52-4, Biphenyl,
 properties 92-62-6, Proflavine 92-71-7, 2,5-Diphenyloxazole
 92-82-0, Phenazine 92-84-2, Phenothiazine 92-87-5, Benzidine
 92-91-1, 4-Acetylbiphenyl 92-94-4, p-Terphenyl 93-04-9,
 2-Methoxynaphthalene 93-08-3, 2'-Acetonaphthone 98-86-2,

Acetophenone, properties 99-98-9, N,N-Dimethyl-p-phenylenediamine 100-06-1 100-22-1, N,N,N',N'-Tetramethyl-p-phenylenediamine 100-23-2, N,N-Dimethyl-4-nitroaniline 100-42-5, Styrene, properties 101-60-0, 21H,23H-Porphine 103-30-0, trans-Stilbene 108-90-7, Chlorobenzene, properties 114-25-0, Biliverdin 116-31-4, all-trans-Retinal 116-85-8, 1-Amino-4-hydroxyanthraquinone 117-79-3, 2-Aminoanthraquinone 118-75-2, Chloranil, properties 119-61-9, Benzophenone, properties 119-65-3, Isoquinoline 120-12-7, Anthracene, properties 120-72-9, Indole, properties 120-73-0, Purine 121-69-7, N,N-Dimethylaniline, properties 121-97-1, 4'-Methoxypropiophenone 122-00-9 122-39-4, Diphenylamine, properties 127-40-2, all-trans-Lutein 127-47-9, Retinyl acetate 128-95-0, 1,4-Diaminoanthraquinone 129-00-0, Pyrene, properties 134-84-9, 4-Methylbenzophenone 134-85-0, 4-Chlorobenzophenone 135-19-3, 2-Naphthol, properties 135-48-8, Pentacene 135-88-6, N-Phenyl-2-naphthylamine 153-78-6, 2-Aminofluorene 190-70-5, Benzo[a]coronene 191-07-1, Coronene 191-13-9, Pyranthrene 191-24-2 192-97-2, Benzo[e]pyrene 195-19-7, Benzo[c]phenanthrene 198-55-0, Perylene 213-46-7, Picene 215-58-7, Benzo[b]triphenylene 217-59-4, Triphenylene 218-01-9, Chrysene 222-93-5, Pentaphene 253-52-1, Phthalazine 256-81-5, 5H-Dibenzo[a,d]cycloheptene 259-79-0, Biphenylene 260-94-6, Acridine 275-51-4, Azulene 290-37-9, Pyrazine 290-87-9, s-Triazine 298-81-7, 8-Methoxypsoralen 302-79-4, all-trans-Retinoic acid 339-16-2, all-trans-Methyl retinoate 345-83-5, 4-Fluorobenzophenone 365-07-1, Thymidine-5'-monophosphate 366-29-0, N,N,N',N'-Tetramethylbenzidine 431-03-8, Biacetyl 472-86-6, 13-cis-Retinal 484-20-8, 5-Methoxypsoralen 486-25-9, Fluoren-9-one 487-06-9, 5,7-Dimethoxycoumarin 492-21-7, 9H-Xanthene-9-thione 492-22-8, Thioxanthen-9-one 492-27-3, Kynurenic acid 494-38-2, Acridine Orange, free base 502-64-7, all-trans-Neurosporene 502-65-8, all-trans-Lycopene 514-73-8, 3,3'-Diethyl-2,2'-thiadibenzocyanine iodide 514-85-2, 9-cis-Retinal 517-51-1, Rubrene 519-62-0, Chlorophyll b 523-27-3, 9,10-Dibromoanthracene 523-50-2, Isopsoralen 527-17-3, Duroquinone 534-97-4, D-Glucose phenylosazone 540-04-5, all-trans-Phytoene 552-82-9, N-Methyldiphenylamine 564-87-4, 11-cis-Retinal 574-93-6, Phthalocyanine 578-95-0, 9(10H)-Acridone 581-89-5, 2-Nitronaphthalene 592-57-4, 1,3-Cyclohexadiene 602-55-1, 9-Phenylanthracene 602-87-9, 5-Nitroacenaphthene 603-17-8, Pheophytin a 603-76-9, 1-Methylindole 604-53-5, 1,1'-Binaphthyl 605-02-7, 1-Phenylanthracene 605-48-1, 9,10-Dichloroanthracene 605-94-7, 2,3-Dimethoxy-5-methyl-1,4-benzoquinone 609-40-5, 2-Nitrothiophene 610-50-4, 1-Anthrol 611-64-3, 9-Methylacridine 611-94-9, 4-Methoxybenzophenone 611-95-0, 4-Carboxybenzophenone 612-78-2, 2,2'-Binaphthyl 612-94-2, 2-Phenylanthracene 613-12-7, 2-Methylantracene 635-65-4, Bilirubin, properties 645-12-5, 5-Nitro-2-furoic acid 709-63-7, 4-(Trifluoromethyl)acetophenone 725-12-2, 2,5-Diphenyl-1,3,4-oxadiazole 728-86-9, 4-(Trifluoromethyl)benzophenone 746-47-4, Bifluorenylidene 771-98-2, 1-Phenylcyclohexene 776-34-1, 1-Amino-4-nitronaphthalene 776-35-2, 9,10-Dihydrophenanthrene 779-02-2, 9-Methylantracene 781-43-1, 9,10-Dimethylantracene 784-04-3, 9-Acetylantracene 796-30-5, 1,4-Diphenylanthracene 824-90-8, β -Ethylstyrene 827-54-3, 2-Vinylnaphthalene 830-81-9, 1-Naphthyl acetate 846-63-9, 2-(1-Naphthyl)-5-phenyloxazole

852-37-9, 2-(4-Biphenyl)-5-phenyloxazole 874-14-6,
 1,3-Dimethyluracil 886-65-7, 1,4-Diphenyl-1,3-butadiene
 904-39-2, 2,2'-(1,4-Phenylene)bisbenzoxazole 905-62-4,
 2,5-Di(1-naphthyl)-1,3,4-oxadiazole 917-23-7,
 meso-Tetraphenylporphine 930-30-3, 2-Cyclopentenone 930-68-7,
 2-Cyclohexen-1-one 958-80-5, 4,4'-Dimethoxythiobenzophenone
 967-72-6 977-96-8, 1,1'-Diethyl-2,2'-cyanine iodide 989-38-8,
 Rhodamine 6G 1065-31-2, Ubiquinone 30 1088-56-8, Lumiflavine
 1107-26-2, β -apo-8'-Carotenal 1146-65-2, Naphthalene-d8
 1204-79-1, 4-Amino-4'-hydroxybiphenyl 1207-72-3,
 N-Methylphenothiazine 1210-12-4, 9-Cyanoanthracene 1217-45-4,
 9,10-Dicyanoanthracene 1220-94-6, 1-Amino-4-(N-
 methylamino)anthraquinone 1226-46-6, 4,4'-
 Bis(dimethylamino)thiobenzophenone 1233-36-9,
 trans-1,2-Bis(1-naphthyl)ethylene 1450-31-3, Thiobenzophenone
 1486-01-7, Biphenyl-d10 1499-10-1, 9,10-Diphenylanthracene
 1517-22-2, Phenanthrene-d10 1522-22-1, 1,1,1,5,5,5-
 Hexafluoroacetylacetone 1564-64-3, 9-Bromoanthracene 1655-29-4
 1661-03-6, Magnesium phthalocyanine 1718-51-0, p-Terphenyl-d14
 1718-52-1, Pyrene-d10 1719-06-8, Anthracene-d10 1720-32-7,
 1,6-Diphenyl-1,3,5-hexatriene 2083-09-2, 2,5-Di(4-
 biphenyl)oxazole 2207-41-2 2216-69-5, 1-Methoxynaphthalene
 2236-60-4, 2-Amino-4-[3H]pteridinone 2257-85-4,
 3-Amino-N-methylphthalimide 2475-44-7, 1,4-
 Bis(methylamino)anthraquinone 2609-46-3, Amiloride 2633-11-6
 2753-11-9, trans-1,2-Bis(2-naphthyl)ethylene 2768-90-3,
 1,1'-Diethyl-2,2'-carbocyanine chloride 2840-87-1,
 trans-1-(1-Naphthyl)-2-phenylethylene 2840-89-3,
 trans-1-(2-Naphthyl)-2-phenylethylene 3029-19-4,
 1-Pyrenecarboxaldehyde 3029-30-9, 1,4-Dicyanonaphthalene
 3029-40-1, 1,8-Diphenyl-1,3,5,7-octatetraene 3071-70-3,
 3,3'-Diethyl-2,2'-thiatricarbocyanine iodide 3117-02-0,
 2,3-Dimethoxy-1,4-benzoquinone 3117-03-1, 2,5-Dimethoxy-1,4-
 benzoquinone 3147-18-0, Pheophytin b 3164-18-9,
 2-(1-Naphthyl)benzoxazole 3591-73-9, 9H-Thioxanthrene-9-thione
 3665-72-3, 5,10-Dihydro-5,10-diphenylphenazine 3902-71-4,
 4,5',8-Trimethylpsoralen 3917-41-7, (E,E)-3-Methyl-5-(2,6,6-
 trimethyl-1-cyclohexen-1-yl)-2,4-pentadienal 3995-46-8
 4237-08-5, 2-Phenyl-2-norbornene 4395-65-7, 1-Amino-4-
 anilinoanthraquinone 4521-90-8, 7,7'-Dihydro- β -carotene
 4727-50-8, 1,1'-Diethyl-4,4'-carbocyanine iodide 4985-70-0,
 1-Chloroanthracene 5121-74-4, 4,4'-Dichlorostilbene 5234-26-4,
 N-(2-Acetylphenyl)acetamide 5257-06-7 5522-63-4,
 Coproporphyrin III, tetramethyl ester 5999-29-1 6345-74-0,
 2-Piperidinoanthraquinone 6406-96-8, 1,5-Dichloroanthracene
 6558-36-7, Benzoylamino-2- Δ^2 -thiazoline
 (extinction coefficient of, global least-squares fit of)
 IT 6963-25-3, 3,3,4,5-Tetraphenyl-2(3H)-furanone 6980-79-6,
 (E,E,E)-5-Methyl-7-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6-
 heptatrienal 6985-27-9, β -apo-14'-Carotenal 7006-08-8,
 Safranin cation 7060-82-4, Methylene Blue cation
 7128-64-5, 2,5-Bis(5-tert-butyl-2-benzoxazolyl)thiophene
 7216-56-0, Neo-alloocimene 7235-40-7, β -Carotene
 7535-48-0, 4',5'-Dihydropsoalalen 10035-62-8, Biliverdin,
 dimethyl ester 10322-23-3, Benz[b]acridin-12(5H)-one
 10355-53-0, 4-Nitro-p-terphenyl 10537-12-9, 9-Phenylacridan
 12581-48-5 13100-79-3, Thiopyronine cation 13638-82-9,
 1,3,6,8-Tetraphenylpyrene 13836-61-8, all-trans-Spheroidene
 13836-70-9, all-trans-Spheroidenone 13920-14-4, 15-cis-Phytoene
 13957-31-8, 4-Thiouridine 14055-21-1, Palladium(II)

etioporphyrin I 14055-23-3, Zinc(II) etioporphyrin I
 14154-42-8 14187-13-4, Palladium(II) tetraphenylporphyrin
 14187-31-6, 1,1'-Diethyl-2,2'-dicarbocyanine iodide 14320-04-8,
 Zinc(II) phthalocyanine 14459-29-1, Hematoporphyrin IX
 14586-52-8, Zinc(II) tetrabenzoporphyrin 14640-21-2, Magnesium
 tetraphenylporphyrin 14643-66-4, Coproporphyrin III
 14806-50-9, 3,3'-Diethyl-2,2'-oxadibocyanine iodide
 14977-07-2, Cadmium(II) tetraphenylporphyrin 15158-62-0,
 Tris(2,2'-bipyridine)ruthenium(II) ion 15164-43-9,
 1,1'-Diethyl-6-bromo-2,2'-cyanine iodide 15546-75-5,
 5,10-Dihydro-5,10-dimethylphenazine 15546-77-7 15577-12-5
 15860-31-8, 2-Fluorenyl phenyl ketone 16083-32-2, Coronene-d12
 16341-52-9, trans-Stilbene-d12 16592-08-8, Benzophenone ketyl
 radical, properties 16834-13-2, Tetrakis(4-pyridyl)porphine
 17064-45-8 17251-70-6, Acridine Orange, conjugate monoacid
 17372-87-1, Eosin 17435-19-7, 10-Methyl-9(10H)-acridinethione
 17777-56-9, Triphenylene-d12 17974-57-1, (E,E,E)-6-Methyl-8-
 (2,6,6-trimethyl-1-cyclohexen-1-yl)-3,5,7-octatrien-2-one
 19111-87-6, 2-Bromotriphenylene 19126-38-6, 3,9-Dimethyl-trans-
 fluorenone 19269-15-9 19361-58-1, 15,15'-cis- β -Carotene
 19631-19-7, Chloroindium(III) phthalocyanine 19840-99-4,
 7-Amino-4-methylcarbostyryl 20073-24-9, 3-Carbethoxypsoralen
 20266-45-9, Erythrosin dianion 20669-52-7 20910-35-4
 21850-35-1, 1-(2-Anthryl)-2-phenylethylene 22021-59-6,
 1,5-Diphenylnaphthalene 22082-92-4, 1-(2-
 Chlorophenyl)naphthalene 22559-71-3 22568-06-5 23648-06-8
 23802-37-1, 1-(2-Anthryl)-2-(2-naphthyl)ethylene
 23802-40-6, 1-(2-Anthryl)-2-(2-thienyl)ethylene
 24437-04-5, Proflavine, conjugate monoacid 24552-22-5
 25239-55-8, Methyl viologen radical cation 25529-00-4,
 (E,E,Z)-6-Methyl-8-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3,5,7-
 octatrien-2-one 25767-20-8, Coproporphyrin I, tetramethyl ester
 25777-43-9, Octaethylporphyrinatotoluenetetrakis(IV) dichloride 26071-73-8,
 4-(4-p-Tetraphenylmethyl)benzophenone 26071-74-9,
 2-([1,1':4',1''-Terphenyl]-4-ylmethyl)triphenylene 26754-93-8,
 Thionine cation 26929-86-2 27876-94-4, α -Crocetin
 28406-56-6, Poly(2-vinylnaphthalene) 29120-23-8, Azure A cation
 31589-99-8 34255-08-8, all-trans-Spirilloxanthin 34533-61-4
 34749-75-2, Acridine-d9 34879-84-0, 1,3-Dimethylindazole
 34880-57-4, 2-tert-Butyl-4-methylindazole 35139-10-7,
 2-Naphthalenamine, conjugate acid 35391-47-0, Oxonine cation
 36005-89-7, Selenine 37381-56-9 38321-60-7 39581-33-4,
 N-(2-Acetylphenyl)-N-methylacetamide 39758-70-8, Rhodamine 6G
 dimer 40603-58-5, Zinc(II) tetrakis(4-N-methylpyridyl)porphyrin
 40882-83-5 40904-90-3 47367-75-9, N,N,N',N'-Tetraethyloxonine
 cation 47780-17-6 51674-11-4, 3,6-Dihydroxyphthalimide
 52647-48-0, N-11-cis-Retinylidene-n-butylamine 52806-22-1,
 1-(4-Chlorophenyl)naphthalene 53172-84-2, α -Methyl- β -
 ethylstyrene 53402-96-3, (E,Z,E)-6-Methyl-8-(2,6,6-trimethyl-1-
 cyclohexen-1-yl)-3,5,7-octatrien-2-one 53402-97-4,
 (E,Z,Z)-6-Methyl-8-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3,5,7-
 octatrien-2-one 54226-17-4, (Z,E)-3-Methyl-5-(2,6,6-trimethyl-1-
 cyclohexen-1-yl)-2,4-pentadienal 55539-00-9, Thionine cation,
 conjugate monoacid 56013-12-8, (E,Z)-3-Methyl-5-(2,6,6-trimethyl-1-
 cyclohexen-1-yl)-2,4-pentadienal 56013-13-9,
 (Z,Z)-3-Methyl-5-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4-
 pentadienal 57704-78-6, 1-(2-Biphenyl)-1-phenylethylene
 58270-06-7, Lumiflavine, conjugate monoacid 59019-35-1,
 N-(2-Acetylphenyl)-N-methylformamide 59728-89-1 59728-91-5
 59729-16-7, Zinc(II) tetrakis(3-N-methylpyridyl)porphyrin

61769-47-9, N-all-trans-Retinylidene-n-butylamine 62399-34-2
 62888-19-1 63415-60-1 63697-27-8, Triphenylamine, conjugate
 acid 64140-99-4, Neomethylene Blue cation 64358-50-5,
 4'-Aminomethyl-4,5',8-trimethylpsoralen 65589-70-0 66610-20-6,
 properties 66933-95-7, 7-Oxa-2,3-dibenzoylbicyclo[2.2.1]hepta-
 2,5-diene 66933-96-8 67024-10-6, (2'-Chlorobenzoyl)amino-2-
 Δ2-thiazoline 67567-20-8 67605-76-9 67777-65-5, Benzyl
 9-anthroate 68716-04-1 69374-19-2 69374-23-8 69374-37-4
 69417-82-9 69458-19-1 70239-57-5 71753-20-3 72225-18-4
 72225-19-5 72618-27-0 72746-33-9, ζ-Carotene 72905-22-7
 73097-13-9, 4',5'-Dihydro-3-carbethoxypsoralen 74007-32-2,
 7-Oxa-2,3-dibenzoylbicyclo[2.2.1]hept-2-ene 79619-74-2
 79745-32-7, Palladium(II) tetrakis(p-sulfonatophenyl)porphyrin
 80863-44-1, Dibromofluorescein dianion 81052-70-2,
 trans-2,3-Dimethyl-2,3-di-(2-naphthyl)oxirane 81052-71-3,
 cis-2,3-Dimethyl-2,3-di-(2-naphthyl)oxirane 81052-72-4,
 trans-2,3-Di-(2-naphthyl)oxirane 81052-73-5,
 cis-2,3-Di-(2-naphthyl)oxirane 81725-25-9,
 Chloro(methanol) (phthalocyaninato) rhodium(III) 81725-26-0,
 Bromo(methanol) (phthalocyaninato) rhodium(III) 81725-27-1
 83364-16-3, Palladium(II) tetrakis(4-N-methylpyridiyl)porphyrin
 84138-95-4 86289-54-5 86289-55-6, 8,9,10,11,12,13,14,15-
 Octahydro-5,7:16,18-dietheno-2,21-octanocyclopentadeca[1,2-a:1,15-
 a']diindene 86289-56-7 86289-57-8 86334-02-3,
 (R)-4-Methoxydinaphtho[2,1-d:1',2'-f[1,3,2]dioxaphosphepin 4-oxide
 87810-82-0 90819-76-4, 11-cis-β-Apo-14'-carotenal
 91036-25-8 91947-21-6, Zinc(II) tetrakis(2,6-dimethyl-4-
 sulfonatophenyl)porphyrin 92000-19-6, Tetrakis(2,6-dimethyl-4-
 sulfonatophenyl)porphine 92545-46-5 96150-36-6 110823-30-8,
 Selenine cation, conjugate monoacid 110823-31-9, Safranine
 cation, conjugate monoacid 110823-32-0, Safranine cation,
 conjugate diacid 110823-33-1, Oxonine cation, conjugate monoacid
 110823-34-2, 9-Phenylproflavine, conjugate monoacid 110823-35-3,
 Brilliant Sulfaflavine anion 110823-36-4, 6,7,8,9-Tetrahydro-4-
 hydroxythiazolo[4,5-h]isoquinoline-7-carboxylate ion 110823-37-5
 110823-38-6 110823-39-7, 2-Amino-3-(4-methoxy-6-
 benzothiazolyl)propionate ion 110839-82-2
 (extinction coefficient of, global least-squares fit of)

L44 ANSWER 38 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:92720 HCAPLUS

DOCUMENT NUMBER: 106:92720

TITLE: Spectral change of TCNQ by capture of
 electrons emitted from conducting polymer
 either by photoexcitation or field application

AUTHOR(S): Takeda, Shinji; Yoshino, Katsumi

CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan

SOURCE: Chemistry Express (1986), 1(7), 435-8

CODEN: CHEXEU; ISSN: 0911-9566

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By light irradiation of a polythiophene film immersed in TCNQ/MeCN
 solution, a remarkable spectral change was observed, which is explained
 in terms of TCNQ- formation by electron capture from the
 polythiophene. Optical recording and switching elements utilizing
 these spectral changes are proposed.

IT 25233-34-5, Polythiophene

(optical absorption by TCNQ/acetonitrile solns. over films of,
 light-induced changes in)

RN 25233-34-5 HCAPLUS

CN Thiophene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1

CMF C4 H4 S



CC 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 74, 76

IT 25233-34-5, Polythiophene

(optical absorption by TCNQ/acetonitrile solns. over films of, light-induced changes in)

IT 1518-16-7, TCNQ

(optical absorption by solns. of, in acetonitrile, over polythiophene film, light-induced changes in)

L44 ANSWER 39 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:135550 HCAPLUS

DOCUMENT NUMBER: 98:135550

TITLE: A novel spectroscopic method for the investigation of structural phase transitions in molecular crystals

AUTHOR(S): Ghoshal, S. K.; Sarkar, S. K.; Kastha, G. S.

CORPORATE SOURCE: Opt. Dep., Indian Assoc. Cultiv. Sci., Calcutta, 700032, India

SOURCE: Molecular Crystals and Liquid Crystals (1983), 91(1-2), 1-24

CODEN: MCLCA5; ISSN: 0026-8941

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple exptl. technique for the investigation of structural phase transitions in mol. crystals at 77-300 K was developed and applied to a wide variety of organic mol. crystals. The Photokinematical Approach, as the method has been termed, utilizes the responsiveness of photoluminescence of guest aromatic ketone mols. to the changes in crystalline structure of host mol. crystals as sensitive probe for the identification of structural phase transformations in host mol. crystals. In this method the prediction of the number of distinct polymorphs, their corresponding optimum temps. of existence, and the transition temps. is based on the observation of characteristic changes in the luminescence intensity of the guest ketone mols. that occur in response to host crystalline modifications. The reliability of the method was established from the conformity and reproducibility of the results the technique yields in its application to a number of well characterized mol. crystals. The results reveal close correlation between the occurrence of structural phase transitions and the occurrence of noncoplanar mol. conformation in polymorphic crystals.

IT 110-02-1

(phase transitions in, spectroscopic method in study of)

RN 110-02-1 HCAPLUS

CN Thiophene (8CI, 9CI) (CA INDEX NAME)



CC 75-7 (Crystallography and Liquid Crystals)

Section cross-reference(s): 73

ST phase transition mol crystal luminescence

IT Luminescence

(of aromatic ketone mols., in mol. crystals, phase transitions of host mol. crystals in relation to)

IT 56-23-5, properties 60-29-7, properties 62-56-6, properties
 65-85-0, properties 85-01-8, properties 92-94-4 95-94-3
 98-86-2, properties 100-02-7, properties 103-33-3 106-46-7
 108-87-2 108-88-3, properties 110-00-9 110-02-1
 110-82-7, properties 110-86-1, properties 118-75-2,
 properties 118-92-3 119-61-9, properties 120-51-4
 129-00-0, properties 134-81-6 290-37-9 290-87-9 504-29-0
 588-59-0

(phase transitions in, spectroscopic method in study of)

L44 ANSWER 40 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1982:590738 HCAPLUS

DOCUMENT NUMBER: 97:190738

TITLE: 30.4 nm Helium(He II) photoelectron spectra of organic molecules. Part VII. Miscellaneous compounds

AUTHOR(S): Bieri, Gerhard; Aasbrink, Leif; Von Niessen, Wolfgang

CORPORATE SOURCE: Phys. Dep., R. Inst. Technol., Stockholm, S-100 44 70, Swed.

SOURCE: Journal of Electron Spectroscopy and Related Phenomena (1982), 27(2), 129-78
 CODEN: JESRAW; ISSN: 0368-2048

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Detailed 30.4-nm He(II) photoelectron spectral data are presented for H₂S, SF₆, SiF₄, cyclopropane, cyclopentadiene, 1,5-hexadiyne, norbornadiene, NH₃, MeNH₂, ethyleneimine, pyrrole, cyanoethylene, 1,2-dicyanoethylene (trans-, cis-, and geminal-), tetracyanoethylene, trans-1,2-fluorocyanoethylene, PhCN, ethylene oxide MeCHO, Me₂O, Me₂CO, furan, thiophene, propiolic acid Me ester, cyclopentanone, 1,4-dioxane, urea, HCONMe₂, propargyl chloride, allyl chloride, allyl bromide, pentafluorohalobenzenes, Cl₂, Br₂, and I₂. The assignment of the observed bands is taken in general from Green's function calcns., in the remaining cases from semiempirical HAM/3 calcns. or from previous studies. The Green's function calcns. give the ionization energy as well as the relative intensity values.

IT 110-02-1
 (UPS of)

RN 110-02-1 HCAPLUS

CN Thiophene (8CI, 9CI) (CA INDEX NAME)



CC 73-6 (Optical, Electron, and Mass Spectroscopy and Other
Related Properties)
IT 57-13-6, properties 67-64-1, properties 68-12-2, properties
74-89-5, properties 75-07-0, properties 75-19-4 75-21-8,
properties 100-47-0, properties 106-95-6, properties
107-05-1 107-13-1, properties 109-97-7 110-00-9
110-02-1 115-10-6 120-92-3 121-46-0 123-91-1,
properties 151-56-4, properties 344-04-7 344-07-0
542-92-7, properties 624-65-7 628-16-0 670-54-2,
properties 764-42-1 827-15-6 922-64-5 922-67-8 928-53-0
2551-62-4 7553-56-2, properties 7664-41-7, properties
7726-95-6, properties 7782-50-5, properties 7783-06-4,
properties 7783-61-1 83218-27-3
(UPS of)

L44 ANSWER 41 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:492904 HCAPLUS
DOCUMENT NUMBER: 73:92904
TITLE: Calculation of excited state and ground state
properties of conjugated heteroatomic
molecules using a single SCF-LCAO-CI method
including σ -polarization
AUTHOR(S): Hammond, Howell A.
CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY,
USA
SOURCE: Theoretica Chimica Acta (1970), 18(3), 239-49
CODEN: TCHAAM; ISSN: 0040-5744
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An SCF- π method including variable π -electronegativity and
 σ -polarization is described and applied to the calcn. of
electronic transitions and ionization potentials of a large
variety of heteroat. mols. containing B, N, O, F, Cl, and S. The
necessary atomic parameters are the Slater effective nuclear
charges and published ionization potentials, electron affinities
and σ -orbital electronegativities for trigonally hybridized
atoms. The program automatically adjusts the initial atomic
parameters to reflect the mol. environment without the
intervention of the user. The agreement between calculated and observed
transition energies, oscillator strengths, and ionization
potentials is very good.
IT 110-02-1, properties
(mol. orbital configuration interaction energy levels of, mol.
consts. in relation to)
RN 110-02-1 HCAPLUS
CN Thiophene (8CI, 9CI) (CA INDEX NAME)



CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic

Resonance, and Other **Optical** Properties)

IT 62-53-3, properties 71-43-2, properties 107-02-8, properties
108-90-7, properties 109-97-7 110-00-9 110-02-1,
properties 110-86-1, properties 462-06-6 497-20-1
(mol. orbital configuration interaction energy levels of, mol.
consts. in relation to)

IT 91-58-7 98-80-6 98-95-3, properties 100-47-0
106-51-4, properties 108-95-2, properties 271-89-6
273-53-0 486-25-9 873-51-8 2622-57-3 13059-59-1
16969-45-2, properties
(mol. orbitals of, mol. consts. in relation to)

L44 ANSWER 42 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:448159 HCAPLUS
DOCUMENT NUMBER: 69:48159
TITLE: Reversible E.P.R. photosignals in
charge-transfer complexes
AUTHOR(S): Ilten, D. F.; Kronenberg, M. E.; Calvin, M.
CORPORATE SOURCE: Lawrence Radiat. Lab., Univ. of California,
Berkeley, CA, USA
SOURCE: Photochemistry and Photobiology (1968), 7(4),
331-40
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Solns. of p-chloranil in 16 organic solvents, of o-chloranil in
thiophene and diphenyl ether, of tetracyanoethylene in diphenyl
ether, pyridine, and EtCl₂, and of perylene in hexafluorobenzene,
were irradiated in a search for rapidly reversible E.P.R.
photosignals. The rise and decay of charge-transfer complex
photosignals for chloranil-containing organic systems were of the order
of tens of msec. The mechanisms involved can only be fully worked
out by using addnl. data, for example flash photolysis results.

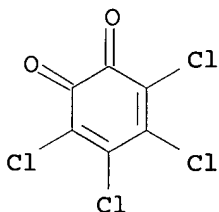
IT 22317-92-6
(electron spin resonance of light-excited)

RN 22317-92-6 HCAPLUS

CN o-Benzoquinone, 3,4,5,6-tetrachloro-, compd. with thiophene (8CI)
(CA INDEX NAME)

CM 1

CRN 2435-53-2
CMF C6 Cl4 O2



CM 2

CRN 110-02-1
CMF C4 H4 S



CC 73 (Spectra and Other **Optical** Properties)
 IT 3470-32-4 20591-11-1 20591-12-2 20591-13-3 20591-14-4
 20591-16-6 20659-29-4 20659-30-7 20721-81-7
 22317-92-6
 (electron spin resonance of light-excited)
 IT 670-54-2, properties
 (electron spin resonance of pyridine solns. of)
 IT 118-75-2, properties
 (electron spin resonance of quinoline solns. of, effect of uv
 irradiation on)

L44 ANSWER 43 OF 43 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1968:55077 HCAPLUS

DOCUMENT NUMBER: 68:55077

TITLE: PR separations of band envelopes produced by
 prolate and oblate top molecules

AUTHOR(S): Seth Paul, Willem A.; Dijkstra, Greult

CORPORATE SOURCE: Res. Lab., Janssen Pharmaceutica n.v., Beerse,
 Belg.

SOURCE: Spectrochimica Acta, Part A: Molecular and
 Biomolecular Spectroscopy (1967), 23(12),
 2861-70

CODEN: SAMCAS; ISSN: 1386-1425

DOCUMENT TYPE: Journal

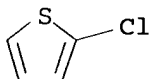
LANGUAGE: English

AB A study of P R sepns. produced by a relatively large number of
 prolate and oblate asym. top mols. reported in the literature
 revealed that under certain conditions the branch sepns. of type
 A(.dblvert.), type B(1), and type C(1) bands (prolate
 mols.) are in the proportion of 1:1/S(β):3/2, whereas the
 sepns. produced by type A(1), type B(1), and type
 C(.dblvert.) bands (oblate mols.) are in the proportion of
 2/3:1/S(β):1 and 2/3:2/3:1 for planar oblate compds. The
 branch separation of the parallel bands is found to obey the relation:
 $\Delta\nu(\text{PR}) = 10S(\beta) (\text{BT}/9)^{1/2} \text{ cm}^{-1}$ For $\rho^* \leq$
 $3/4$ and $-1 \leq \nu\kappa \leq +1$ the proposed .cxa.x
 values fairly match those as calculated by Gerhard and Dennison and by
 Badger and Zumwalt as well. The method of predicting branch
 sepns. is therefore simplified while the agreement with the values
 observed by experiment is quite satisfactory. 71 references.

IT 96-43-5
 (spectrum (ir) of, in gas phase, separation of PR band envelopes in)

RN 96-43-5 HCAPLUS

CN Thiophene, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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 (spectrum (ir) of, in gas phase, separation of PR band envelopes in)